

N₂O isotope approaches for source partitioning of N₂O production and estimation of N₂O reduction – validation with ¹⁵N gas-flux method in laboratory and field studies

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Table S1: Summary of mixing endmembers isotopic signatures of particular pathways (bD- bacterial denitrification, nD- nitrifier denitrification, fD- fungal denitrification, Ni- nitrification) and reduction fractionation factors (reduction) with respective references (ref.). For the model input each value is corrected with the respective mean isotopic signature of the substrate: for $\delta^{18}\text{O}$ – soil water ($\delta^{18}\text{O}_{\text{H}_2\text{O}}$) for bD, nD and fD, for $\delta^{15}\text{N}$ – respective substrate – NO_3^- for bD and fD and NH_4^+ for nD and Ni, with distinct values applied for field ($\delta^{15}\text{N}_{\text{field}}$ for F1, F2, F3) and laboratory ($\delta^{15}\text{N}_{\text{lab}}$ for L1, L2) studies. The respective substrate corrected values were applied as a model input for $\delta^{18}\text{O}$ and $\delta^{15}\text{N}$, for $\delta^{15}\text{N}^{\text{SP}}$ no substrate correction is needed. The final model input values are marked with green bold font.

pathway	literature values				substrate isotope values			substrate corrected values		
	$\delta^{15}\text{N}^{\text{SP}}$	$\delta^{18}\text{O}$	$\delta^{15}\text{N}$	ref.	$\delta^{18}\text{O}_{\text{H}_2\text{O}}$	$\delta^{15}\text{N}_{\text{field}}$	$\delta^{15}\text{N}_{\text{lab}}$	$\delta^{18}\text{O}$	$\delta^{15}\text{N}_{\text{field}}$	$\delta^{15}\text{N}_{\text{lab}}$
bD	-1.9±4.6	19.0±2.1	-45.8±4.7	¹⁻⁶	-6.4	11.9	4.5	12.6±2.1	-33.9±4.7	-41.3±4.7
nD	-5.9±6.5	15.7±2.9	-56.9±3.8	^{4,7}	-6.4	41.4	79.3	9.3±2.9	-15.5±3.8	22.4±3.8
fD	33.6±2.5	46.9±3.8	-38.0±6.6	^{3,8-10}	-6.4	11.9	4.5	40.5±3.8	-26.1±6.6	-33.5±6.6
Ni	35.0±2.9	23.5±2.1	-57.0±7.3	^{4,7,11,12}		41.4	79.3		-15.6±7.3	22.3±7.3
reduction	-6.0±1.4	-15.9±4.7	-7.0±2.1	^{2,13-17}						

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Table S2: Comparison of SP/O Map results of all calculation cases (Case 1 and Case 2) and mixing scenarios (bD-fD and bD-Ni).

		$r_{\text{N}_2\text{O}}$				f_{bD}			
scenarios		bD-fD		bD-Ni		bD-fD		bD-Ni	
cases		Case1	Case2	Case1	Case2	Case1	Case2	Case1	Case2
L1	min	0.15	0.14	0.14	0.14	0.96	0.79	0.98	0.84
	max	0.24	0.24	0.26	0.24	1	1	1	1
	mean	0.19	0.18	0.19	0.18	0.99	0.93	0.99	0.95
L2	min	0.16	0.15	0.16	0.16	0.94	0.88	0.96	0.91
	max	0.52	0.53	0.45	0.46	1	1	1	1
	mean	0.27	0.27	0.25	0.25	0.98	0.96	0.99	0.97
F1	min	0.68	0.70	0.44	0.48	0.62	0.55	0.81	0.66
	max	1.00	1.00	0.76	0.77	0.84	0.83	0.91	0.87
	mean	0.86	0.86	0.62	0.64	0.74	0.70	0.86	0.77
F2	min	0.30	0.36	0.22	0.27	0.84	0.64	0.94	0.73
	max	0.43	0.49	0.38	0.39	0.95	0.89	0.97	0.92
	mean	0.38	0.42	0.29	0.32	0.92	0.77	0.96	0.83
F3	min	0.26	0.27	0.25	0.25	0.97	0.92	0.98	0.94
	max	0.47	0.47	0.46	0.46	1	1	1	1
	mean	0.33	0.32	0.32	0.32	0.99	0.97	0.99	0.98

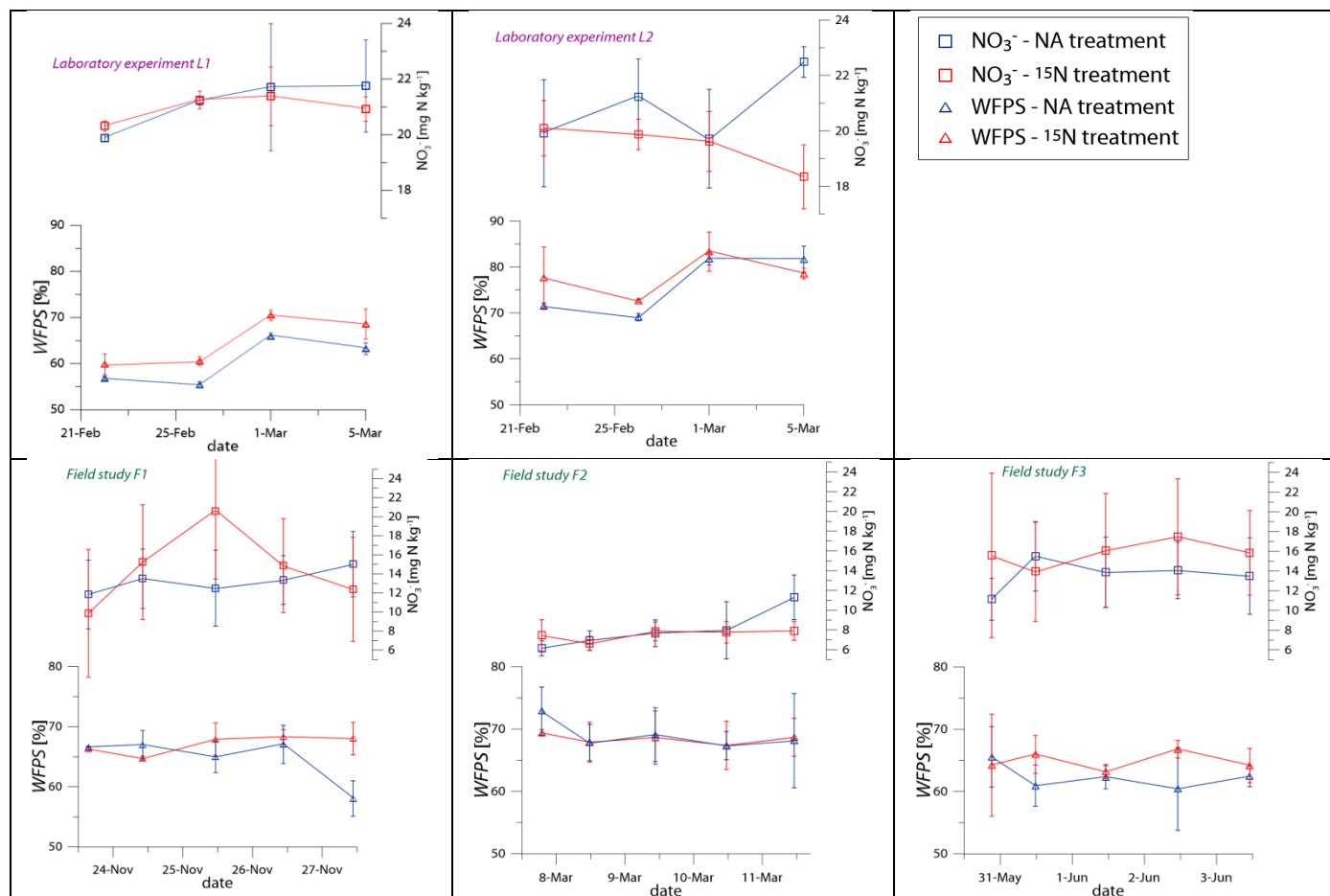


Fig. S1 Soil conditions during laboratory incubations and field campaigns. Water filled pore space (WFPS in %) and nitrate content in mg N kg⁻¹ dry soil is shown for NA treatment (blue symbols) and ¹⁵N treatment (red symbols). Note different Y-Axis scaling for laboratory and field studies.

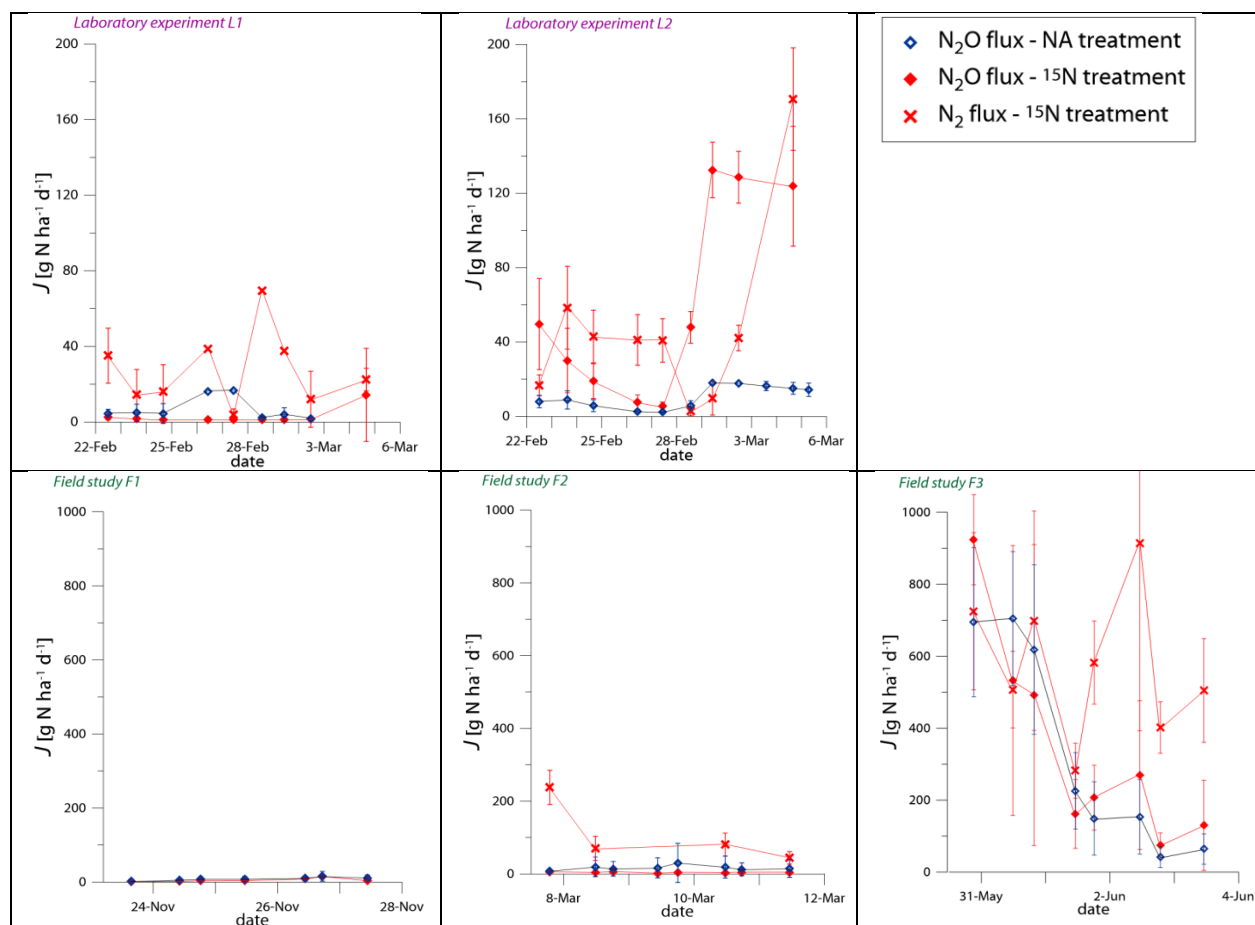


Fig. S2 Gas fluxes in $\text{g N ha}^{-1} \text{d}^{-1}$. Note different Y-Axis scaling for laboratory and field studies. Mean values for each sampling date with standard deviation ($n=4$) are shown. N₂O flux (diamonds) in NA treatment (blue symbols) and ¹⁵N treatment (red symbols) and N₂ flux determined in ¹⁵N treatment is shown (red crosses).

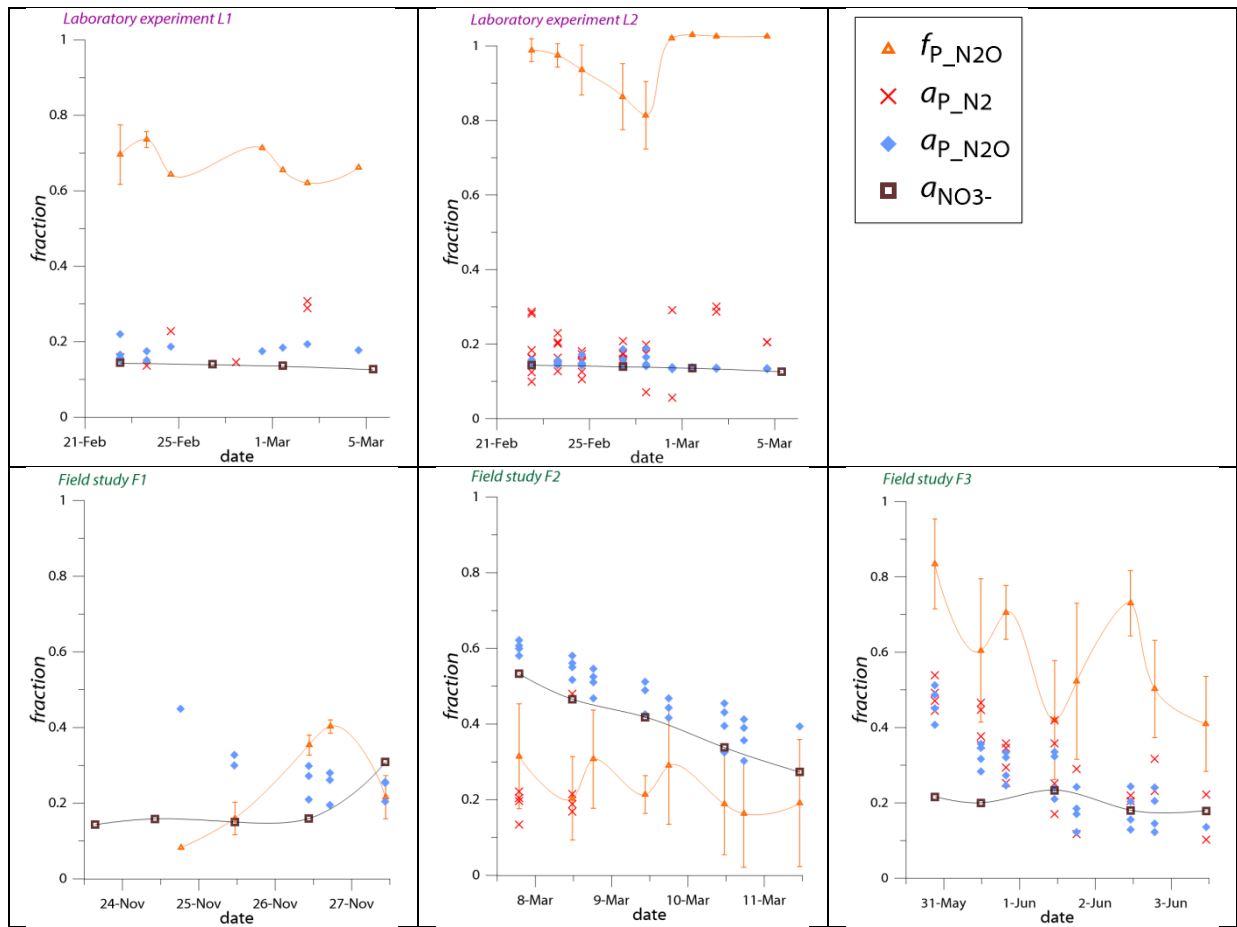
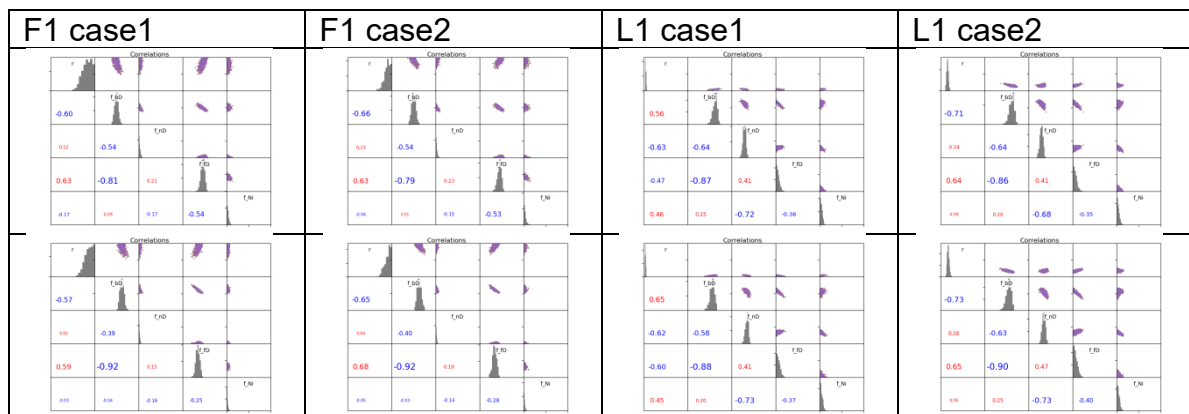
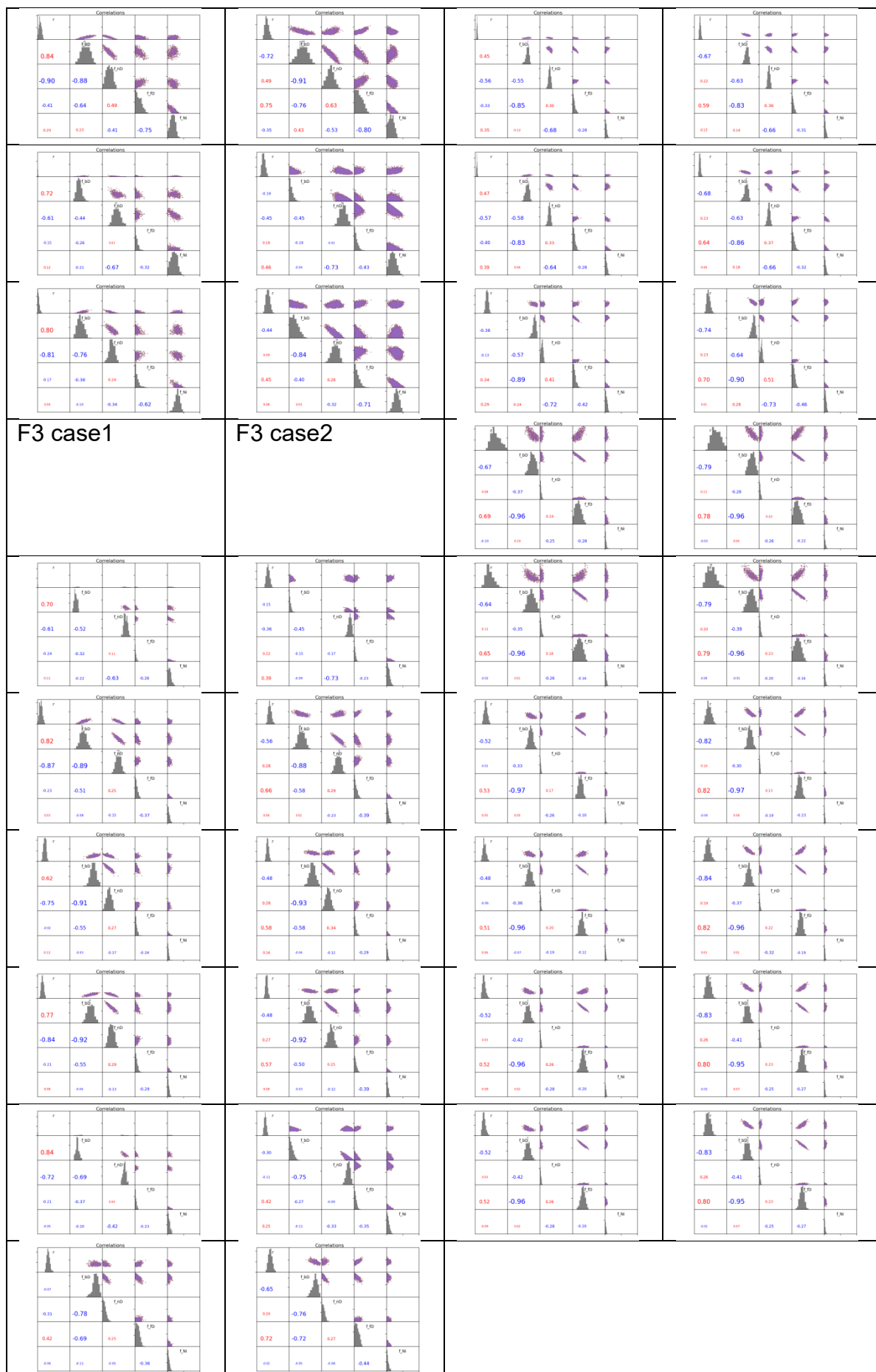


Fig. S3 ^{15}N abundance in total NO_3^- ($a_{\text{NO}_3^-}$ – brown squares), NO_3^- pool producing N_2O ($a_{\text{P_N}_2\text{O}}$ – blue diamonds), NO_3^- pool producing N_2 ($a_{\text{P_N}_2}$ – red crosses) and ^{15}N pool-derived fraction of N_2O ($f_{\text{P_N}_2\text{O}}$ – orange triangles). For $a_{\text{NO}_3^-}$ and $f_{\text{P_N}_2\text{O}}$ mean values for each sampling date with standard deviation ($n=4$) are shown. For $a_{\text{P_N}_2}$ and $a_{\text{P_N}_2\text{O}}$ all individual values are shown (due to numerous missing data).





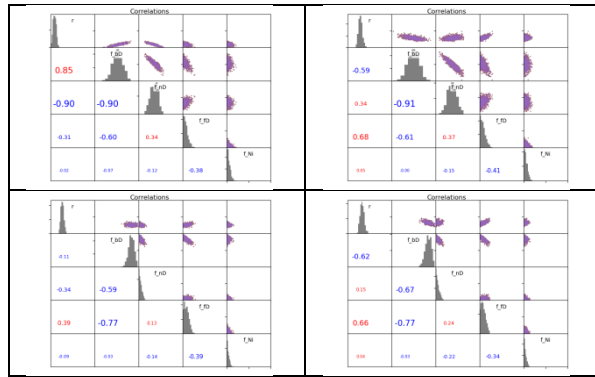


Fig. S4 Matrix plots presenting detailed 3DI model outputs for each sampling date for both calculating cases. The plots in the diagonal show histograms of posterior probability distribution of r_{N2O} and mixing fractions, the plots above the diagonal show correlations between the modeled fractions and the values below the diagonal show R coefficient of these correlations: in blue for positive correlations and in red for negative correlations with the size proportional to the R value.