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Disentangling the rates of carbonyl sulfide (COS) production and consumption and their dependency on soil properties across biomes and land use types

Aurore Kaisermann et al.

Correspondence to: Aurore Kaisermann (aurore.kaisermann@inra.fr)

SiteID	pH	Redox	Bulk density	Vol.Water	WFPS	Clay	Silt	Sand	Soil C	Soil N	CaCO$_3$	Phosphate	MBC	MBN	CO2 dried soil
	(-)	(mV)	(g.cm-3)	(cm^3.cm^{-3})	(-)	(g.kg^{-1})	(g.kg^{-1})	(g.kg^{-1})	(g.kg^{-1})	(g.kg^{-1})	(g.kg^{-1})	(ugP.mL)	(ug.g^{-1})	(ug.g^{-1})	(umol.m2.s^{-1})
FI-Hyy	4.4	410	0.51	0.23	0.28	138	317	545	98	2.73	20	0.17	1056	120	0.0
FI-Var1	5.2	305	0.76	0.11	0.16	44	168	788	28	0.89	14	0.00	135	14	0.3
FI-Var2	4.9	341	0.76	0.15	0.21	NA	NA	NA	NA	NA	NA	NA	546	73	0.3
SE-Hyl	3.9	433	0.52	0.12	0.15	142	346	512	105	4.11	20	0.69	851	110	0.0
SE-Nor	4.6	309	0.56	0.20	0.26	133	260	607	74	2.36	20	0.52	1139	120	0.0
SE-Ros2	4.9	314	0.85	0.12	0.18	35	148	817	16	0.38	14	0.01	100	9	0.0
SE-Ros1	4.3	348	0.81	0.12	0.17	40	303	657	21	0.79	20	0.00	107	8	0.0
SE-Sva	4.2	400	0.54	0.21	0.27	86	282	632	85	2.17	7	1.32	918	115	0.1
ES-Amo	8.5	239	0.93	0.12	0.19	145	345	510	28	1.49	4	0.12	1030	110	-0.4
ES-Bal	8.5	180	0.89	0.10	0.15	180	275	545	20	1.56	9	0.11	650	57	-0.3
ES-Ube1	8.6	168	0.86	0.12	0.17	548	401	51	71	1.51	16	0.13	835	70	0.0
ES-Ube2	8.4	185	0.99	0.12	0.19	NA	NA	NA	NA	NA	NA	NA	671	47	0.0
IL-Reh	7.9	191	1.01	0.15	0.24	147	67	786	14	0.79	13	0.16	362	31	-0.1
IL-Yat	8.6	192	0.87	0.16	0.24	288	490	222	58	1.92	9	0.25	1214	142	-0.3
PT-Cor	5.8	257	1.13	0.11	0.20	37	155	808	12	0.68	1	0.34	165	16	0.0
PT-Mit	6.0	257	0.80	0.11	0.15	40	85	875	17	0.95	20	0.34	479	52	0.0
CH-Cha	5.5	371	0.70	0.16	0.21	282	441	277	25	2.61	14	1.10	961	84	0.0
CH-Dav	4.2	407	0.33	0.21	0.24	221	254	525	144	5.34	14	0.17	1450	145	0.0
CH-Fru	4.8	377	0.74	0.18	0.26	238	446	316	42	4.07	1	0.14	903	98	0.0
CH-Lae	6.3	277	0.75	0.19	0.27	423	425	152	37	2.81	3	0.16	724	10	0.0
CH-Oe2	6.9	248	0.89	0.17	0.26	416	469	115	28	2.77	6	0.31	552	43	-0.3
DE-Hai	5.7	292	0.87	0.25	0.37	476	485	39	39	3.05	14	0.10	677	-17	0.0
DE-Lei	5.0	380	0.88	0.15	0.23	187	772	41	31	2.33	7	0.03	542	55	0.0
DK-Sor	4.2	371	0.63	0.17	0.22	149	234	617	56	2.97	14	0.26	572	58	0.1
FR-Hes	5.1	331	0.87	0.18	0.26	244	610	146	22	1.56	20	0.01	509	52	0.0
FR-Lqu1	4.2	420	0.54	0.16	0.20	179	594	227	95	9.07	1	0.02	1012	28	0.0
FR-Lqu2	4.9	383	0.55	0.22	0.28	206	579	215	113	10.23	1	0.03	2302	190	0.0

Table S1: Table summarising the soil properties for the 27 soils used in this study (n=3). Vol.Water is the volumetric water content, Soil C and Soil N are the soil total C and N concentrations, MBC and MBN are the microbial biomass C and N, CO$_2$ dried soil are the CO$_2$ fluxes measured using the method 1 on air-dried soils.

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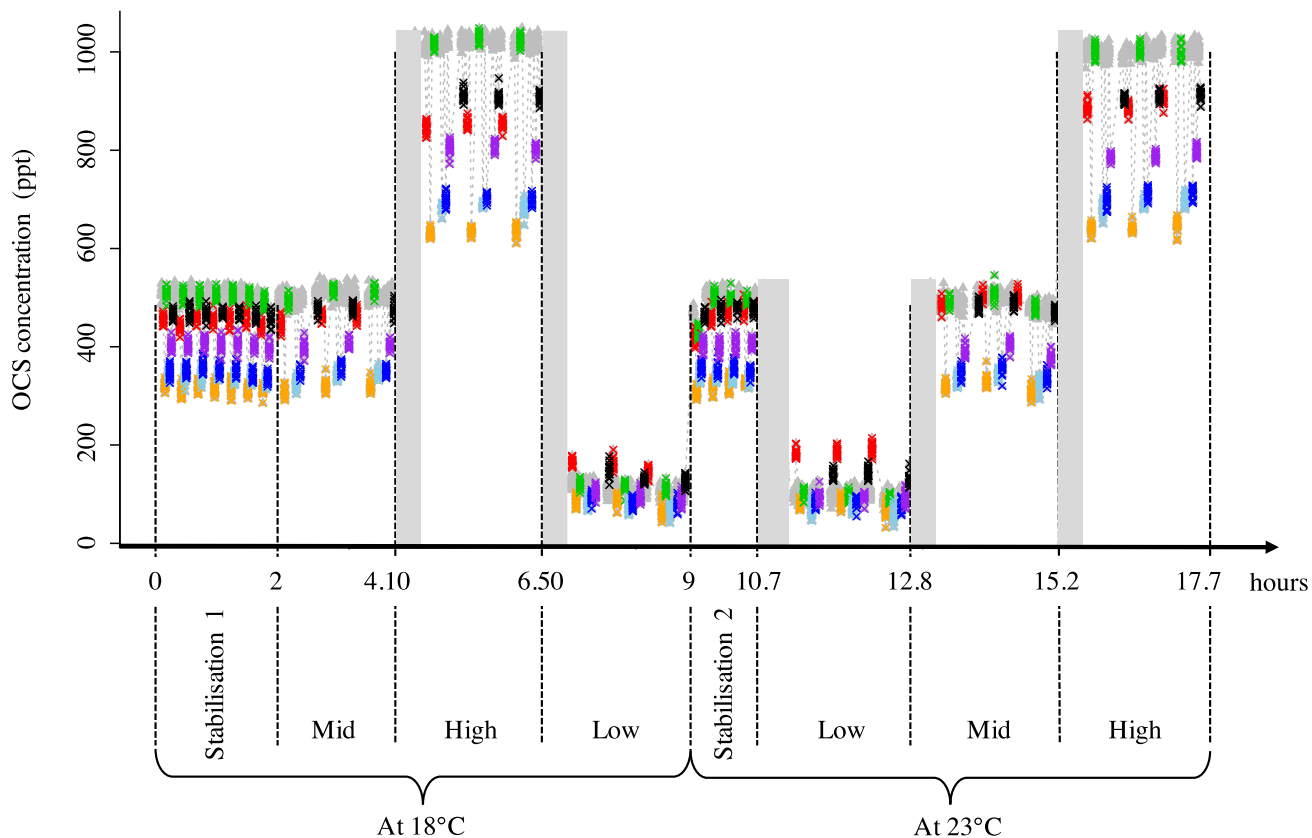
Figure S2: Sequence of gas exchange measurements programmed to measure the net COS exchange for Method 2. The measurement of COS concentration was done for gas entering in the jars (grey cross) in alternating for gas exiting the six jars with soils (red, orange, skyblue, blue, purple and black) and the empty jar (green). The measurement was realised every second for 120 seconds, only the last 15 seconds (each single cross) were used for average. The measurements were done three times for each jar, at three levels of COS concentration entering in the pots (Low, Mid and High) at two temperature levels (18°C and 23°C). The jars were connected to the measurement system for two hours to equilibrate gas between soil and atmosphere (Stabilisation 1). The measurements done during the 30 minutes after changing the level of COS concentration (grey rectangle) and 1h45 after changing the temperature in the climatic chamber (Stabilisation 2) were not used for analysis to assure sufficient time to have stable gas fluxes.

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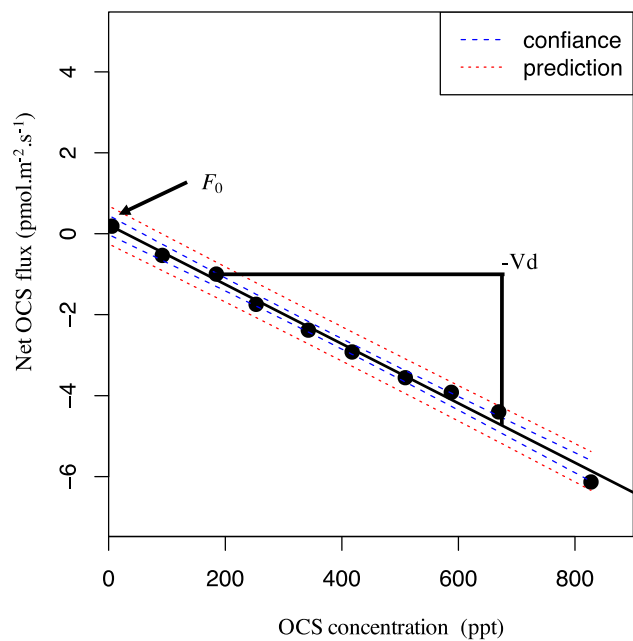
Figure S3: Determination of the gross production rate when the net COS flux at zero of COS concentration (F_0) and the pseudo-first order uptake rate constant (Vd) by measuring the flux of COS as function of the COS concentration over soil in a flow-through system (adapted from Conrad 1994). Black line is the linear model, blue line is the confidence interval and red lines is the prediction interval.

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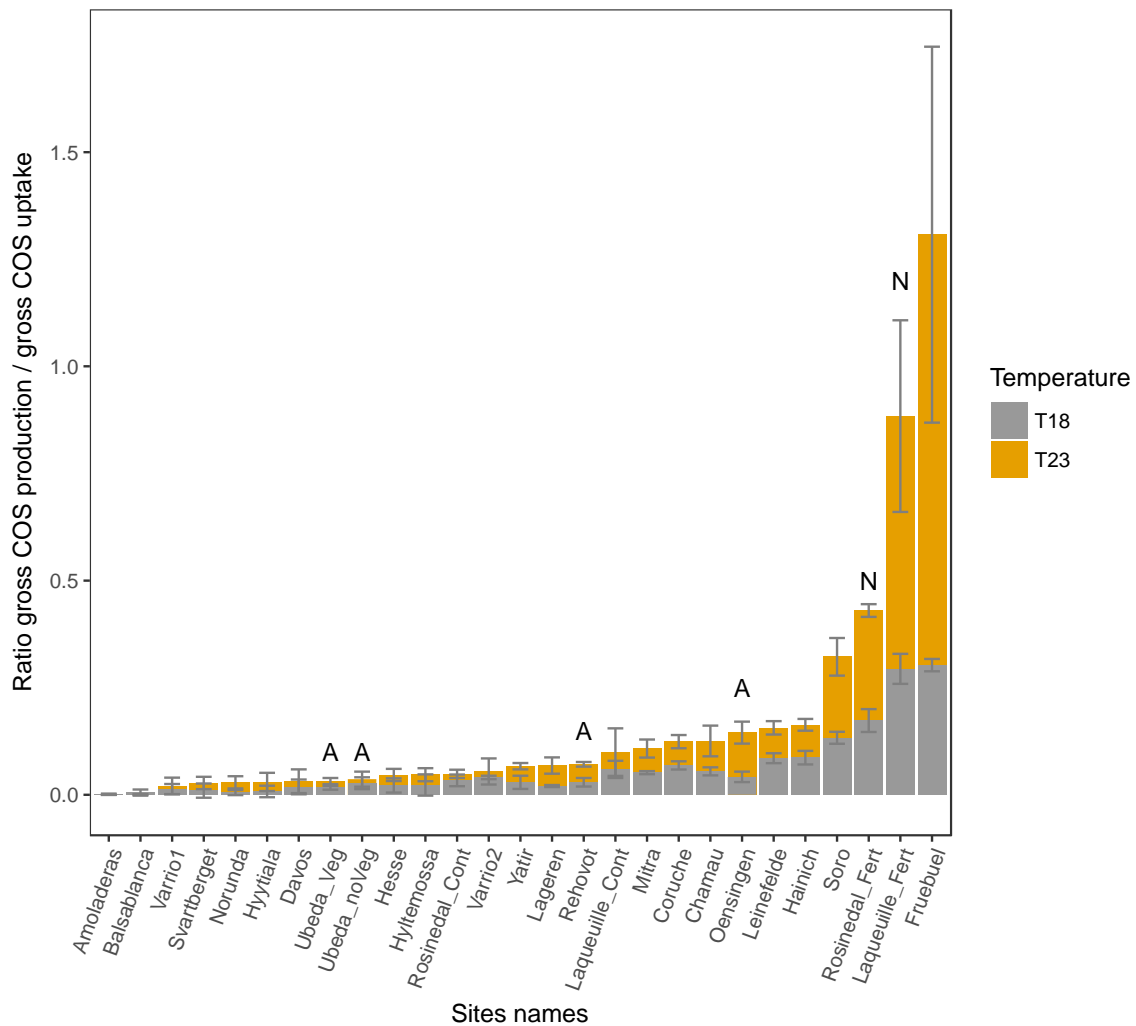
Figure S4: The ratio of gross COS source to the gross COS uptake in the 27 soils (n=3 ± sd) at 18°C and 23°C. Agrosystem sites are highlighted using the letter A and experimentally fertilised sites with the letter N to compare with unfertilized plots at the same site.
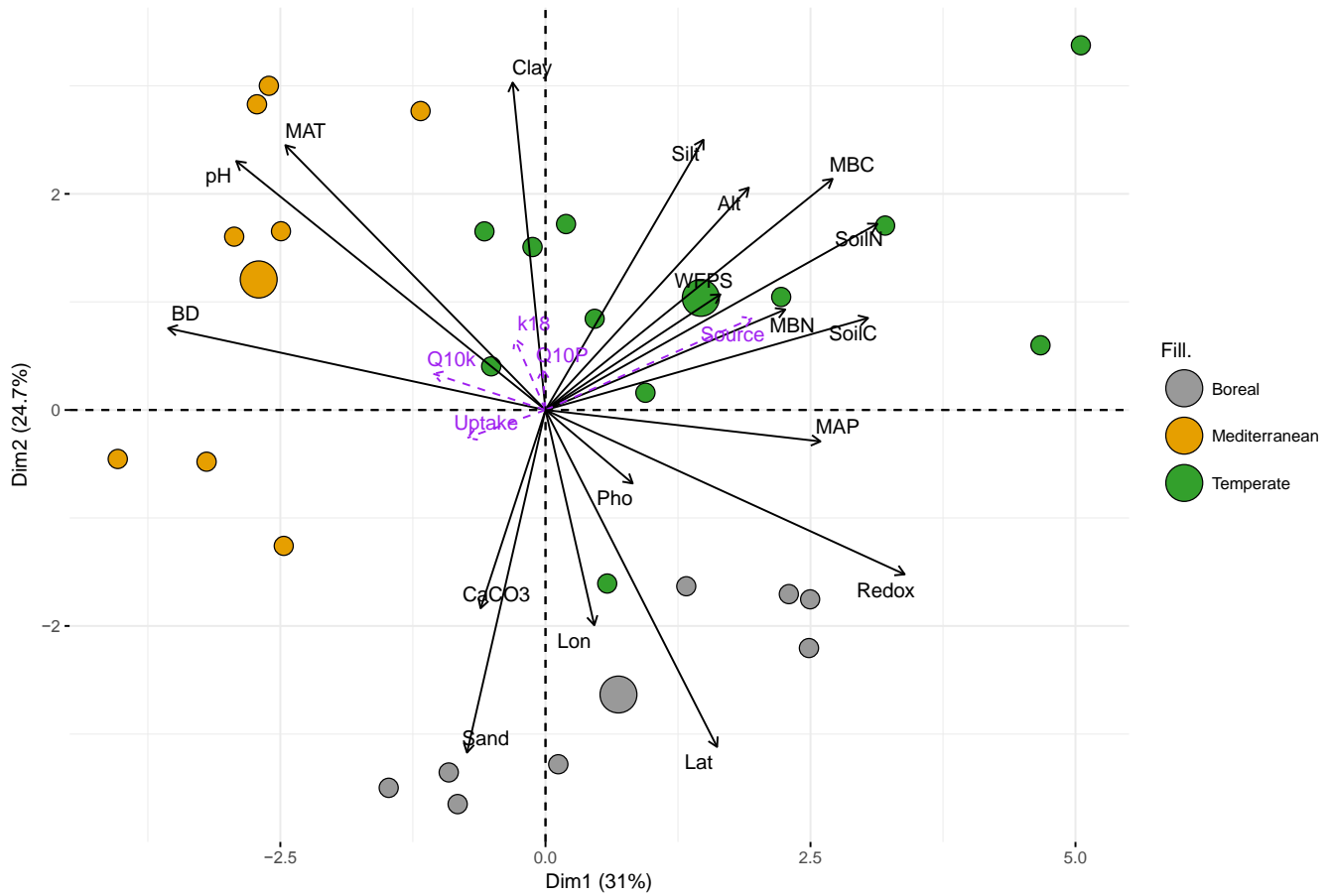
Figure S5: Biplot principal component analysis (PCA) of the 27 soils in this study. Each small point represents the mean of the three replicates of one soil coloured by the biome (Boreal, Mediterranean, Temperate), the big points represent the barycentre of each biome. Black arrows are the active variables (standardized physico-chemical properties) used to build the PCA (BD= Bulk density; MBC and MBN = microbial biomass carbon and nitrogen; WFPS = water filled pore space, Alt = altitude, Lon=longitude, Lat=Latitude, MAT= mean annual temperature, MAP= Mean annual precipitation, Pho=Phosphate content).

To investigate the inter-relations between COS fluxes and soil properties, variables of COS fluxes (Source = gross OCS production at 18°C; uptake = gross OCS uptake at 18°C; Q10k and Q10P = Q_{10} of hydrolysis rate and of the source; and k18= first-order hydrolysis rate constant at 18°C) were fitted as supplementary variables into the PCA using the package R called FactoMineR. The purple arrows are the supplementary variables with the coordinates projected onto the PCA and predicted using only the information provided by the performed PCA on active variables.

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