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Supplement of

Challenges in soil carbon modelling and measurement: a decade of experimental data vs. RothC simulations in an organic olive grove

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Table S1. Summary of SOC observations excluded using the MAD filtering procedure

Sampling date	Treatment	Total observations *(n)*	Excluded observations *(n)*	Removed *(%)*	Excluded SOC values *(Mg·ha^{-1})*	Median SOC *(Mg·ha^{-1})*	MAD
nov-13	Control	3	1	33	40.56	31.68	8.75
jul-17	Control	3	1	33	20.16	31.2	5.25
may-23	Control	6	1	17	81.12	38.4	4.82
nov-23	Control	6	1	17	105.9	42.04	11.64
may-24	Control	6	1	17	86.12	41.38	4.02
jul-14	Compost	3	1	33	76.32	47.4	4.32
may-15	Compost	3	1	33	88.56	45.96	5.62
sep-16	Compost	3	1	33	33.36	37.56	5.33
jul-17	Compost	3	1	33	37.92	51.12	4.08
jul-22	Compost	6	1	17	102.48	46.66	6.33
jul-23	Compost	6	2	33	92.64; 64.56	151.8	20.04; 29.79
nov-23	Compost	6	1	17	95.76	57.94	6.31
mar-24	Compost	6	2	33	152.64; 91.44	56.46	15.22; 5.22
nov-13	Mixture	3	1	33	54.24	41.8	518.99
jul-14	Mixture	3	1	33	48.96	63.61	203.99
may-15	Mixture	3	1	33	135.84	57.48	11.59
sep-16	Mixture	3	1	33	34.08	47.88	7.71
nov-21	Mixture	6	1	17	41.76	54.48	4.87
jul-22	Mixture	6	1	17	104.64	47.904	5.45
nov-23	Mixture	6	1	17	122.88	53.712	5.47
mar-24	Mixture	6	1	17	134.16	69.84	5.92
may-24	Mixture	6	1	17	134.16	81.264	4.96
jun-13	Biochar	3	1	33	38.4	109.38	13.26
may-15	Biochar	3	1	33	197.52	73.2	18.00
sep-16	Biochar	3	1	33	37.92	70.92	6.74
nov-21	Biochar	6	1	17	84.96	47.184	6.57
may-23	Biochar	6	1	17	120.48	70.464	5.50
jul-23	Biochar	6	1	17	186.72	103.54	4.67
nov-23	Biochar	6	1	17	118.08	68.4	5.68
mar-24	Biochar	6	2	33	125.28; 122.64	65.7	7.38; 7.03

Total observations: number of SOC measurements per sampling date; Excluded observations: number of measurements removed after MAD filtering; % Excluded: percentage of excluded observations; Excluded SOC values: SOC measurements identified as outliers; Median SOC: median SOC value after filtering; MAD: Median Absolute Deviation used as the outlier detection criterion.

Table S2. Main characteristic of the compost used in incubation experiment on a dry weight basis, and RothC model input data and parameters used for the inversion procedure.

EOM	Co-S1	Co-S2	Co-S3
Feedstock	Olive Mill Waste Sheep Manure Olive Tree Pruning	Olive Mill Waste Sheep Manure Olive Tree Pruning	Olive Mill Waste Sheep Manure Olive Tree Pruning
TOC (%)	36.6	36.6	36.6
C/N	16.4	16.4	16.4
pH	8.75	8.75	8.75
WSC_{org} (%)	2.86	2.86	2.86
Soil location	Jaén	Jumilla	Santomera
C Added ($\mu g \cdot g^{-1}$)	6222	6222	6222
BD ($Mg \cdot m^{-3}$)	1.54	1.54	1.53
Clay (%)	13.7	6.5	14.4
Temp (°C)	25	25	25
$DPM \cdot RPM^{-1}$	0.25	0.25	0.25
Depth (cm)	20	20	20
Time (days)	63	63	51

Co-S: Compost-Soil; EOM: Exogenous Organic Matter; TOC: Total Organic Carbon; WSC_{org}: Water-Soluble organic Carbon; C Added: C added to soil by EOM at the beginning of incubation; BD: Bulk Density; $DPM \cdot RPM^{-1}$: ratio between Decomposable Plant Material and Resistant Plant Material required by RothC model; C released: TOC released as CO2 at the final of incubation.

Table S3. Phases of the historical spin-up procedure and relative data.

Phase	Land use	Start (year)	End (year)	Duration (years)	EOM application *($Mg\ C \cdot ha^{-1}$)*	Target SOC *($Mg\ C \cdot ha^{-1}$)*
Spin up reference	Crop generic	997	1997	1000	0	16.17
Transition	Olive orchard	1997	2013	17	1.71	31.36

Table S4. Summary of Aboveground Biomass Density (AGBD) estimated from remote sensing models and used to derive plant carbon inputs (PI) for the RothC simulations under the different treatments. AGBD average corresponds to the mean value of all remote sensing predictions, whereas PI represents the annual plant carbon inputs applied in the simulations. The PI obtained at the end of the historical transition phase (1997–2013) were assumed to represent the PI for the first year of the experiment (2013). Thereafter, PI values were recalculated annually based on changes in AGBD, allowing plant inputs to vary over time according to the estimated development of the olive grove.

Year	AGBD average	Control		Compost		Mixture		Biochar	
		AGBD	PI	AGBD	PI	AGBD	PI	AGBD	PI
	$Mg·ha^{-1}$	*$Mg·ha^{-1}$*	*$Mg\ C·ha^{-1}$*	*$Mg·ha^{-1}$*	*$Mg\ C·ha^{-1}$*	*$Mg·ha^{-1}$*	*$Mg\ C·ha^{-1}$*	*$Mg·ha^{-1}$*	*$Mg\ C·ha^{-1}$*
2013	15.87 *±0.54*	16.62	0.42	16.03	0.42	15.23	0.42	15.60	0.42
2014	15.05 *±0.45*	15.45	0.39	15.01	0.40	14.80	0.41	14.92	0.41
2015	15.45 *±0.18*	15.68	0.40	15.54	0.41	15.19	0.42	15.40	0.42
2016	14.84 *±0.34*	15.15	0.39	14.83	0.39	14.59	0.41	14.79	0.40
2017	15.28 *±0.40*	15.76	0.40	15.32	0.41	14.94	0.42	15.10	0.41
2018	16.10 *±1.18*	16.40	0.42	16.00	0.42	15.44	0.43	16.56	0.45
2019	17.04 *±1.33*	17.96	0.46	16.93	0.45	16.15	0.45	17.11	0.47
2020	18.51 *±0.69*	18.44	0.47	18.30	0.49	18.30	0.51	18.98	0.52
2021	27.04 *±3.28*	27.58	0.70	29.02	0.77	24.26	0.68	27.30	0.74
2022	18.28 *±1.98*	19.25	0.49	18.05	0.48	16.85	0.47	18.97	0.52
2023	23.94 *±1.41*	24.74	0.63	24.52	0.65	21.93	0.61	24.55	0.67
2024	17.52 *±2.03*	18.06	0.46	17.28	0.46	16.95	0.47	17.78	0.48
	x̄ = 17.91	x̄ = 18.42	Σ = 5.65	x̄ = 18.07	Σ = 5.75	x̄ = 17.05	Σ = 5.71	x̄ = 18.09	Σ = 5.91

AGBD: mean Aboveground Biomass Density estimated by the remote sensing model for each treatment; PI: estimated annual carbon input to the soil derived from plant biomass and used in the RothC simulations.

Table S5. Summary of Soil Organic Carbon (SOC) concentrations for soil samples measured in the field experiment through the total experiment duration. These results represent the Mean Standard Deviation (mean Std.Dev), the Mean Standard Error (Mean SE) and mean Coefficient of Variation (CV) for all replicates.

Treatment	Mean Std.Dev *($g·100g^{-1}$)*	Mean SE *($g·100g^{-1}$)*	Mean CV *(%)*	SOC increase *($g·100g^{-1}$)*	SOC rate increase *($g·100g^{-1}·yr^{-1}$)*	Final SOC *($g·100g^{-1}$)*
Control	0.27	0.11	16.85	0.49	0.04	1.80
Compost	0.34	0.14	15.51	1.25	0.11	2.56
Mixture	0.37	0.16	15.54	1.54	0.14	2.84
Biochar	0.46	0.20	15.63	1.71	0.16	3.01

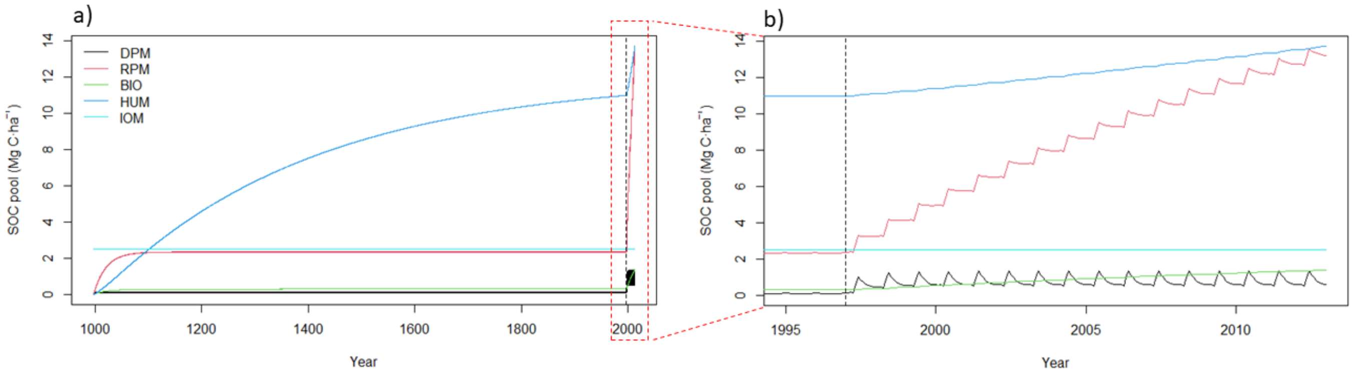

Figure S1. SOC pool sizes during the historical spin-up procedure used for model initialization. In the first stage (a), the model was run for 1000 years under equilibrium conditions to obtain stabilized SOC pool sizes for the land use preceding the 1997 transition, assuming a SOC stock at equilibrium of 16.17 Mg C ha^{-1}. The SOC stock at equilibrium for this stage was measured in an area near the experimental site with the same conditions (soil and land use) as the experimental area before the transition to orchard. In the second stage (b), the model was run from 1997 to 2013 to represent the transition to olive orchard, incorporating a compost input of 1.71 Mg C ha^{-1} y^{-1}. In this stage C plant inputs to the soil were iteratively varied to reach a SOC stock of 31.36 Mg C ha^{-1} as measured at the start of the experimental period.

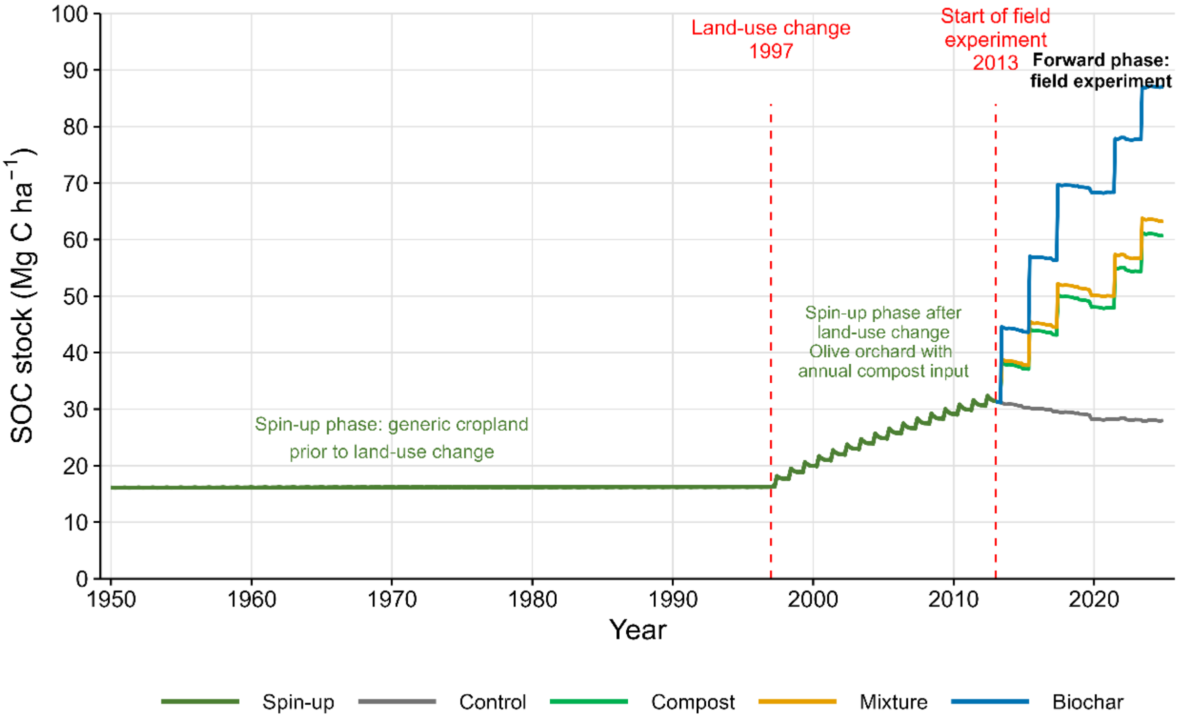

Figure S2. SOC stock dynamics simulated with RothC from the spin-up period to the end of the field experiment. The spin-up phase includes a generic cropland period before land-use change and an olive orchard period with annual compost input, used to initialize SOC pools before the forward simulations. Red dashed vertical lines mark the land-use change in 1997 and the beginning of the field experiment in 2013. Simulated SOC trajectories after 2013 are shown for the Control, Compost, Mixture and Biochar treatments.

Supplementary Information Text

Model inversion procedure for EOM pools' parameterization

Fitting the simulated curve of cumulative CO_2 flux to the measurement from incubations requires an optimization method that searches for the simulation minimizing the discrepancies with observed data. To achieve this, the Differential Evolution Adaptive Metropolis (DREAM) R package (Vrugt et al., 2009a) was used for solving the optimization task in RothC (Scharnagl et al., 2010). This method uses Monte Carlo Markov Chain (MCMC) combined with evolutionary algorithms, improving the accuracy of the solutions and effectively handling high-dimensional problems with multiple solutions (Vrugt et al., 2009b). For the Exogenous Organic Matter (EOM) optimization task, the aim is to estimate a reliable size for each pool and its decomposition rate.

EOM were incubated in Mediterranean soils, specifically from the south of Spain, and the samples were collected at 20 cm depth. The soils employed in incubations were three, so, the materials were named by the number of compost and the type of soil. Table S1 shows the different materials for the soil analysed.

RothC requires the following parameters for performing the simulation: EOM added (Mg C · ha^{-1}), soil clay content (%), temperature (°C), DPM/RPM ratio, depth (cm), and experiment time (days). Table S1 displays the main parameters in the incubation experiment.

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