ORCHIDEE-SOM: Modeling soil organic carbon (SOC) and dissolved organic carbon (DOC) dynamics along vertical soil profiles in Europe

Supplementary material

1. Statistical relationship for K_D based on soil properties

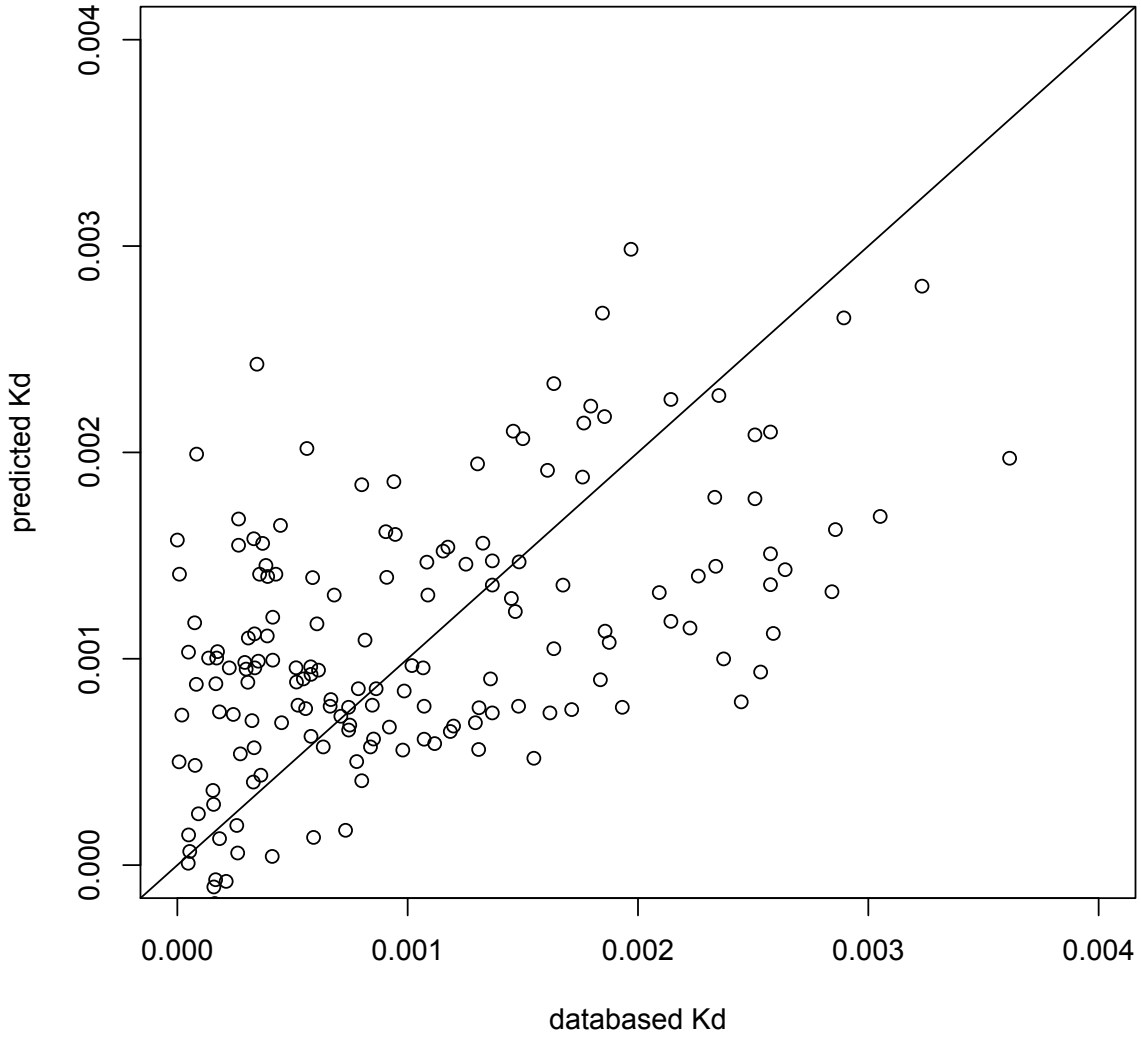

Figure S1. Measured (Kaiser et al., 1996) and modelled (Eq. 15 in manuscript) distribution coefficient K_D as a function of clay and pH. The line is the 1:1 line.

2. Measured versus modelled soil water content (SWC)

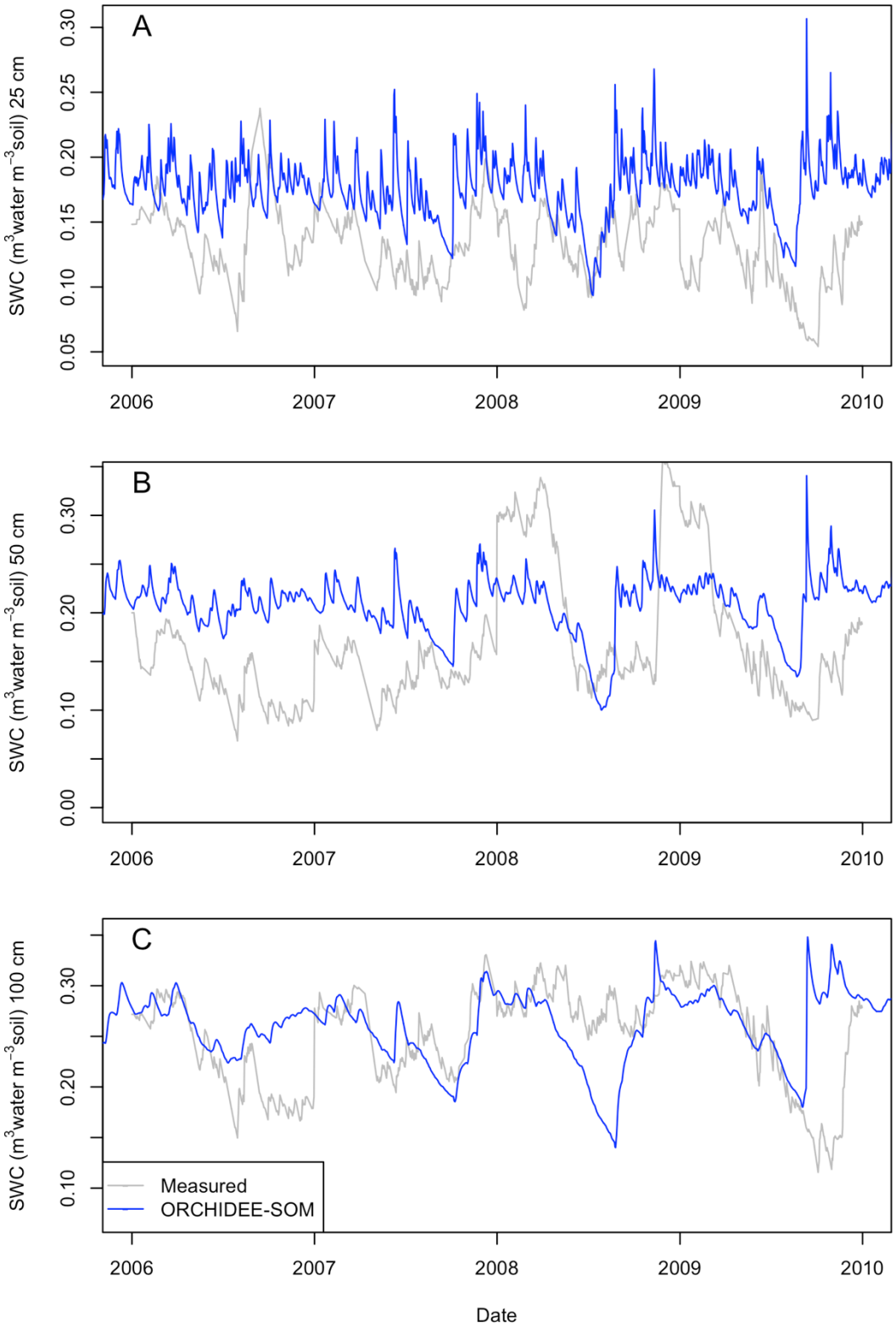

Figure S2. Measured versus modelled soil water content (SWC) for Brasschaat at three soil depths: A) 25 cm, B) 50 cm, C) 100 cm

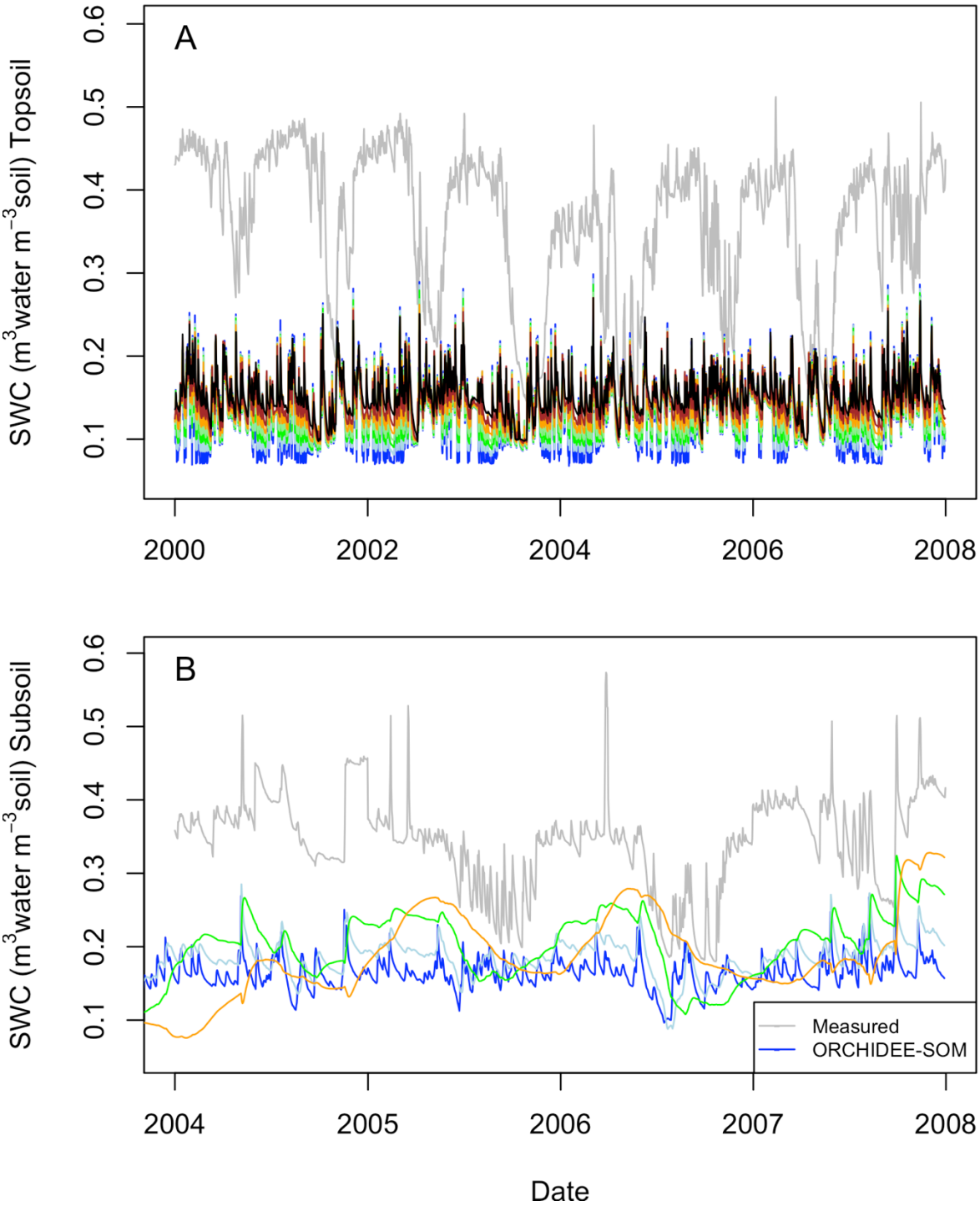

Figure S3. Measured (from FLUXNET dataset) versus modelled soil water content (SWC) for Hainich at two different horizons: A) Topsoil, B) Subsoil. Different colours show SWC modelled by ORCHIDEE from 0 to 20 cm for the topsoil and from 20 to 200 cm for the subsoil.

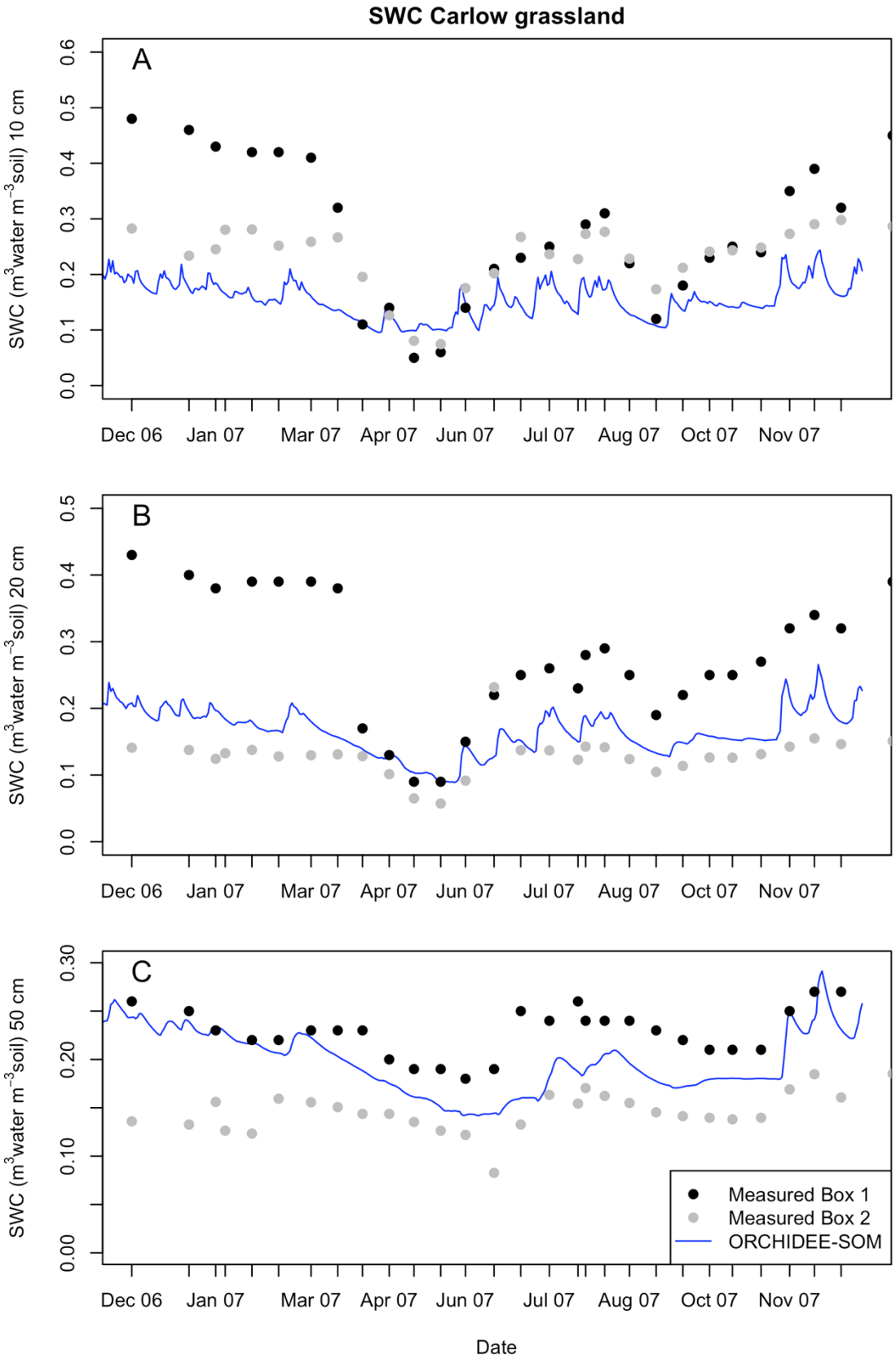

Figure S4. Measured versus modelled soil water content in Carlow grassland at three depths: A) 10 cm, B) 20 cm, C) 50 cm

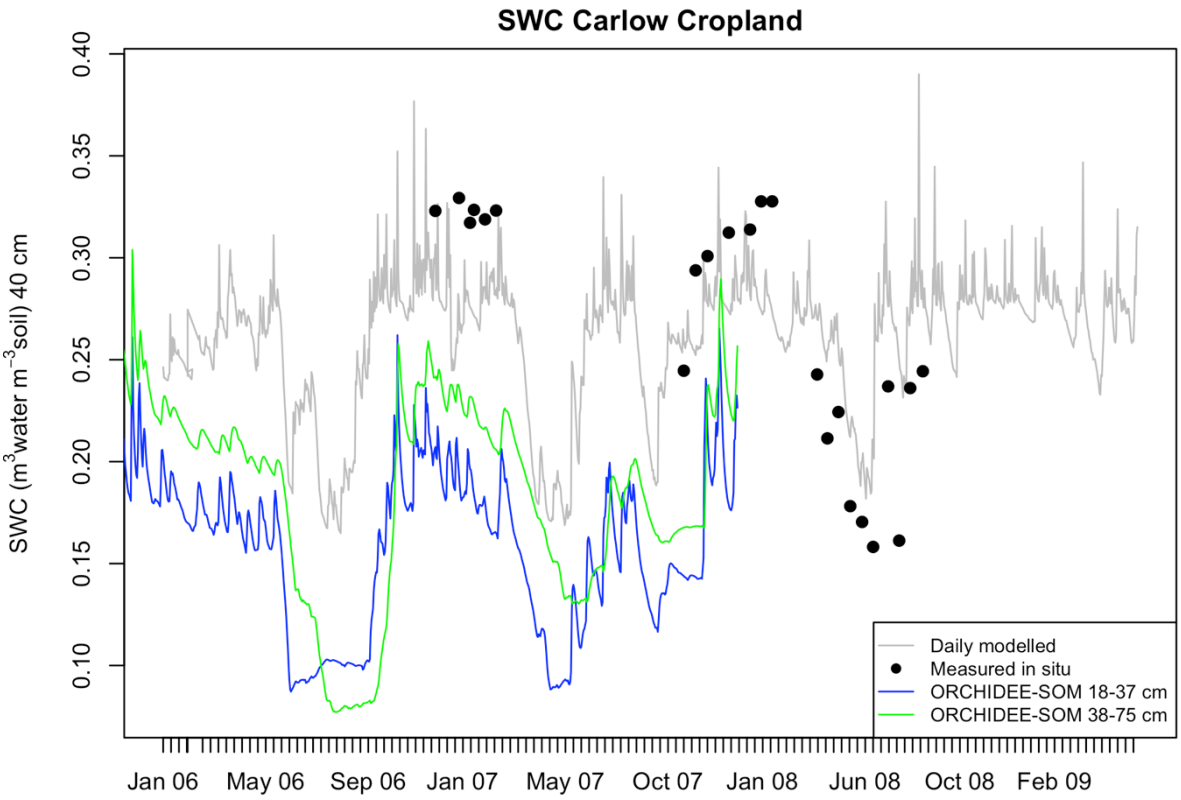

Figure S5. Measured versus modelled soil water content in Carlow cropland. The grey line indicates the soil water content modelled using a soil capacity soil water model (Kindler et al., 2011; Walmsley et al., 2011)

3. Optimization of the GPP-related parameters

Table S1. Values of the optimized parameters before and after the optimization.

Site	Parameter	Prior value	Optimized value
Braaschaat	Maximum LAI	5.0	6.81
	Threshold of LAI below which plant uses carbohydrate reserves	0.5	0.42
	Specific Leaf Area	0.009	0.014
	Maximum temperature for photosynthesis	55.0	57.22
	Minimum temperature for photosynthesis	-4.0	0.93
	Maximum rate of Rubisco activity-limited carboxylation at 25°C	35.0	23.57
Hainich	Maximum LAI	5.0	6.24
	Threshold of LAI below which plant uses carbohydrate reserves	0.5	0.66
	Specific Leaf Area	0.026	0.032
	Maximum temperature for photosynthesis	55.0	57.02
	Minimum temperature for photosynthesis	-4.0	-6.03
	Maximum rate of Rubisco activity-limited carboxylation at 25°C	55.0	38.87
Carlow Cropland	Maximum LAI	5.0	3.26
	Threshold of LAI below which plant uses carbohydrate reserves	0.5	0.40
	Specific Leaf Area	0.026	0.018
	Maximum temperature for photosynthesis	55.0	54.18
	Minimum temperature for photosynthesis	-4.0	-3.95
	Maximum rate of Rubisco activity-limited carboxylation at 25°C	70.0	55.46

4. RMSE and NRMSE values

Table S2. Comparison of mean monthly DOC (mg L^{-1}) and standard deviations (%) from measurements and from ORCHIDEE-SOM. The root-mean-square error (RMSE) and the normalized root-mean-square error (NRMSE) by the mean value of the measurements are reported. The goodness of fit classification is based on criteria described in section 2.3.3.

Site	Depth (cm)	Mean measured DOC	SD measurements	Mean modelled DOC	RMSE	NRMSE (%)	Goodness of fit
Brasschaat	10	39.2	31	127.3	89.3	227.8	Bad
Brasschaat	35	30.4	31	33.7	10.5	34.5	Good
Brasschaat	75	22.3	19	9.9	13	58.3	Fair
Hainich	5	16.7	34	17.5	5	29.9	Very good
Hainich	10	9.2	34	5.5	5.4	58.7	Good
Hainich	20	6.6	57	3.1	5.5	83.3	Good
Carlow Grassland Box 1	10-30	8.5	31	13.3	5.6	65.9	Fair
Carlow Grassland Box 1	60-75	3.6	26	2.8	1.4	38.9	Good
Carlow Grassland Box 2	10-30	14.2	28	13.3	4.75	33.5	Good
Carlow Grassland Box 2	60-75	6.3	24	2.8	3.1	49.2	Good
Carlow Cropland	30-40	4.2	23	4	1.2	28.6	Good
Carlow Cropland	30-40	4.2	23	1.6	3	71.4	Fair

5. Model sensitivity to parameter changes

In order to test the sensitivity of the model to the SOC and DOC residence times and diffusion coefficients, we perform a set of simulations varying such parameters (Table S1). The selection of the parameter values is based on literature or prior knowledge.

Table S3. Parameter values used for each simulation of the sensitivity test

Simulation	CUE	DOC_ TAU	Carbon_tau_ active	Carbon_tau_ slow	Carbon_ta u_passive	Dif	D_DOC
Reference (default)	0.5[1]	1.3[2]	1	6	462	2.74E-7	1.0627E-5
CUE2	**0.35**	1.3	1	6	462	2.74E-7	1.0627E-5
DOC_TAU2	0.5	**60**	1	6	462	2.74E-7	1.0627E-5
Carbon_tau_acti ve2	0.5	1.3	**0.149**	6	462	2.74E-7	1.0627E-5
Carbon_tau_slow 2	0.5	1.3	1	**3**	462	2.74E-7	1.0627E-5
Carbon_tau_pass ive2	0.5	1.3	1	6	**241**	2.74E-7	1.0627E-5
Dif2	0.5	1.3	1	6	462	**1e-6**	1.0627E-5
D_DOC	0.5	1.3	1	6	462	2.74E-7	**1e-4**

[1]Except for Hainich, where the default CUE is 0.35 and for the simulation CUE2, CUE is 0.5

[2]Except for Brasschaat, where the default DOC_TAU is 60 and for the simulation DOC_TAU2 is 1.3

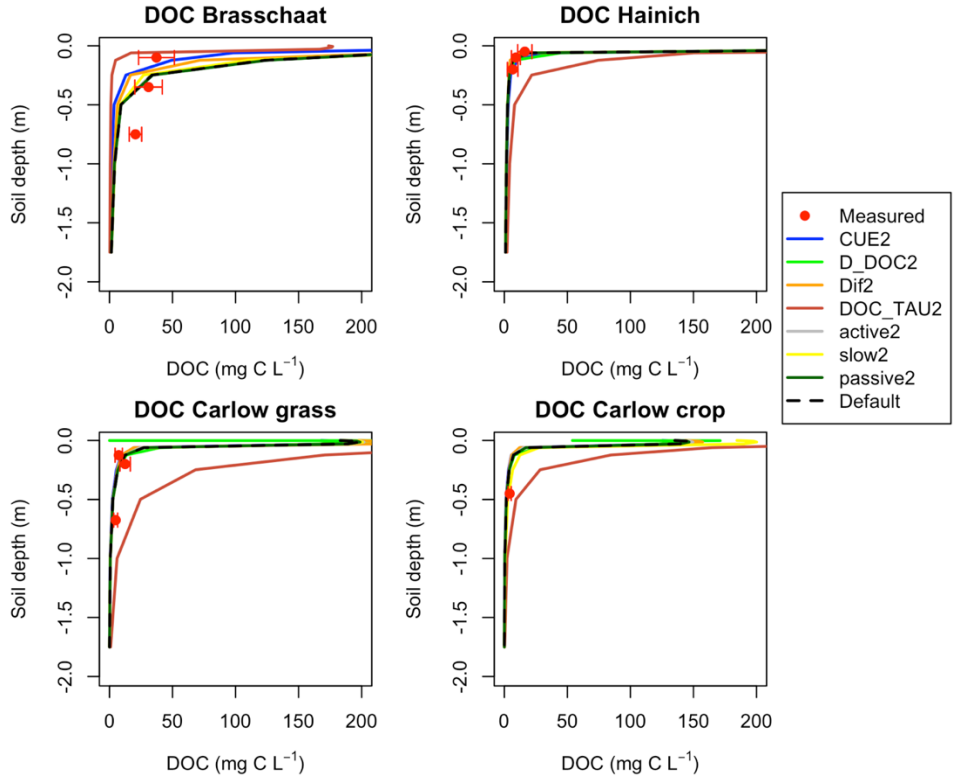

Figure S6. DOC concentrations along the soil profile simulated by the 7 sensitivity tests at the 4 studied sites.

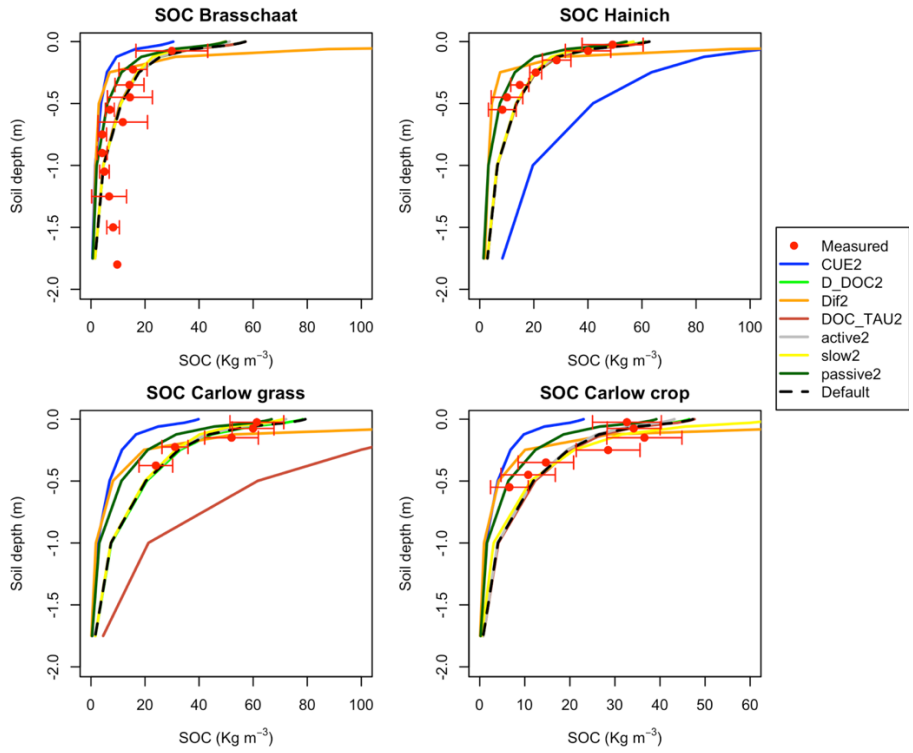

Figure S7. SOC stocks along the soil profile simulated by the 7 sensitivity tests at the 4 studied sites.

References

Kindler, R., Siemens, J., Kaiser, K., Walmsley, D. C., Bernhofer, C., Buchmann, N., Cellier, P., Eugster, W., Gleixner, G., Grunwald, T., Heim, A., Ibrom, A., Jones, S. K., Jones, M., Klumpp, K., Kutsch, W., Larsen, K. S., Lehuger, S., Loubet, B., McKenzie, R., Moors, E., Osborne, B., Pilegaard, K., Rebmann, C., Saunders, M., Schmidt, M. W. I., Schrumpf, M., Seyfferth, J., Skiba, U., Soussana, J. F., Sutton, M. A., Tefs, C., Vowinckel, B., Zeeman, M. J. and Kaupenjohann, M.: Dissolved carbon leaching from soil is a crucial component of the net ecosystem carbon balance, Glob. Chang. Biol., 17(2), 1167–1185, doi:DOI 10.1111/j.1365-2486.2010.02282.x, 2011.

Walmsley, D. C., Siemens, J., Kindler, R., Kirwan, L., Kaiser, K., Saunders, M., Kaupenjohann, M. and Osborne, B. A.: Dissolved carbon leaching from an Irish cropland soil is increased by reduced tillage and cover cropping, Agric. Ecosyst. Environ., 142(3), 393–402, doi:10.1016/j.agee.2011.06.011, 2011.