Supplementary material to: “Modeling the vertical soil organic matter profile using Bayesian parameter estimation”

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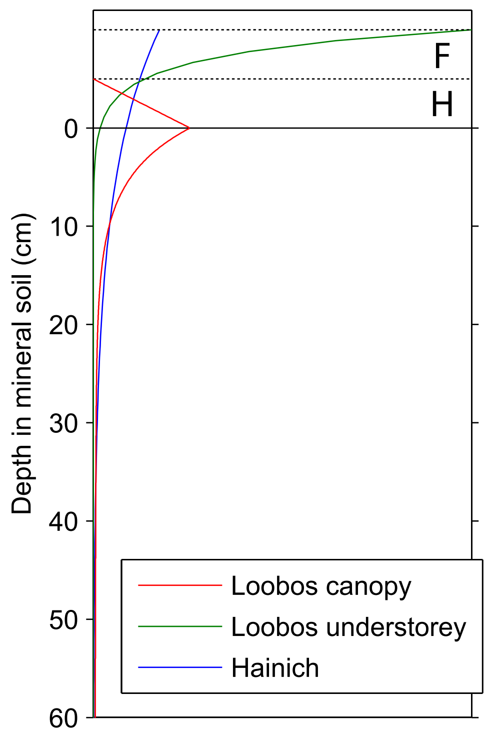

Figure 1: Vertical distribution of the root litter input for Loobos and Hainich used in the simulations. For Loobos different distribution functions were used for the canopy and understorey. The canopy distribution function consists of two parts: a linearly increasing function from zero to 1.0384 from the top to the bottom of H horizon for the organic layer; and a two-term exponential function for the mineral soil: $f(z) = \exp(-20.00\,z) + 0.0384\exp(-0.886\,z)$ (with z the depth in the mineral soil in m). For the understorey at Loobos, and all root input at Hainich, a single-term exponential function starting at the top of the F horizon was used ($f(z) = \exp(-40\,z)$ for Loobos; $f(z) = \exp(-7\,z)$ for Hainich). All curves are normalized so that the integral equals 1.

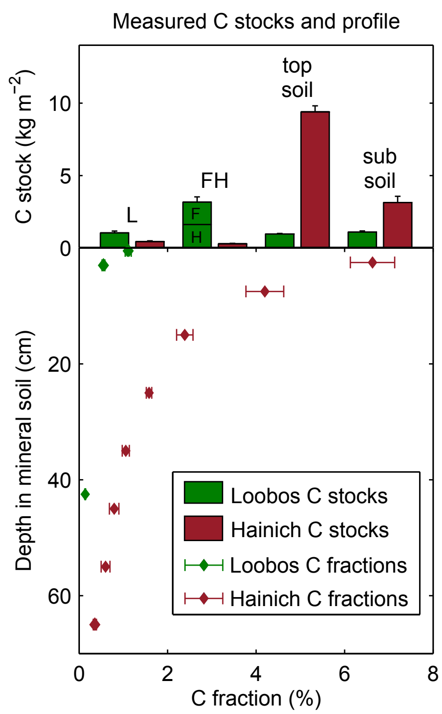

Figure 2: Measured organic carbon stocks and mass fractions at Loobos and Hainich. All quantities are means. Errorbars indicate one standard error of the mean.

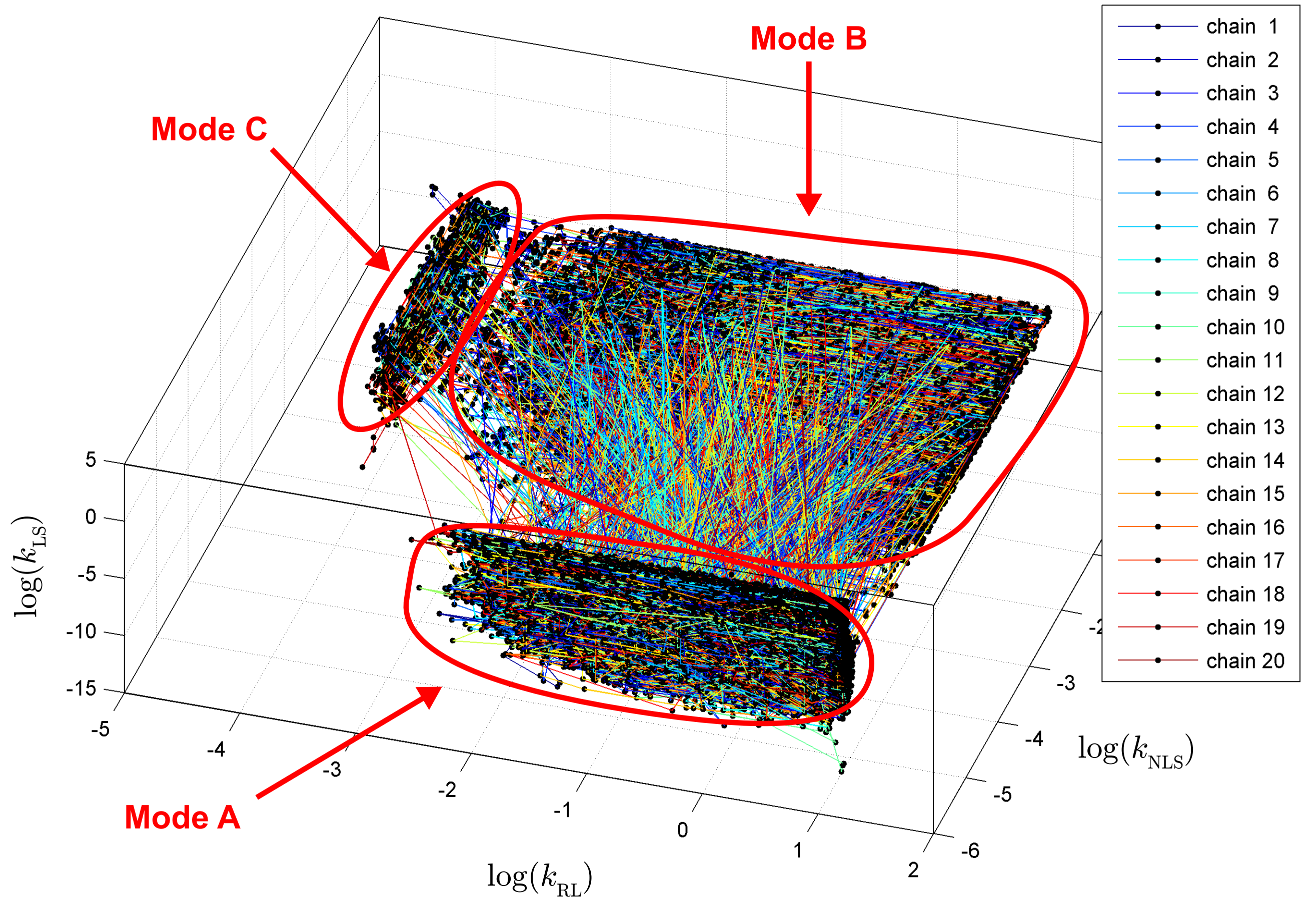

Figure 3: Trace plot of 20 chains sampling the three modes for Hainich for calibration setup 3. The sample was obtained in a supplementary run with the DREAM(ZS) algorithm, estimating only the parameters that differ significantly between the modes: k_{RL}, k_{NLS}, k_{LS} and v (not shown). All other parameters were fixed at the average over the three modes. The variance of the distribution was artificially inflated by a factor 5. The chains were started widely dispersed in the parameter space using Latin hypercube sampling, and were run for 200,000 iterations. The algorithm converged for all parameters (Gelman-Rubin index ≤ 1.01). The many lines between the modes indicate the chains jumping back and forth between them.

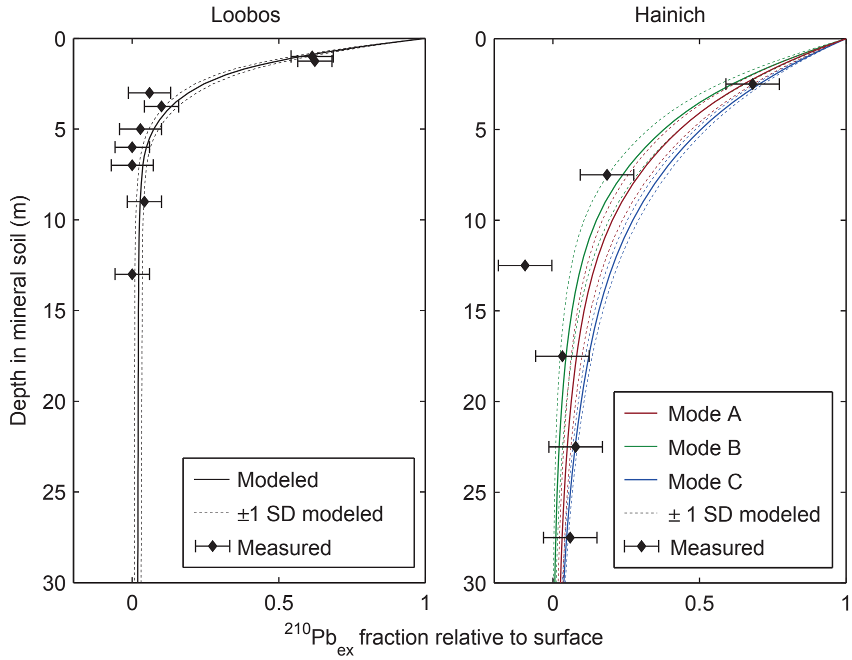

Figure 4: Measured $^{210}Pb_{ex}$fractions relative to surface and corresponding model results for both sites, calibration setup 3. Model results are averages and standard deviations over the Monte Carlo ensemble. Note that the observed $^{210}Pb_{ex}$profile was not measured at Loobos but at an equivalent site.

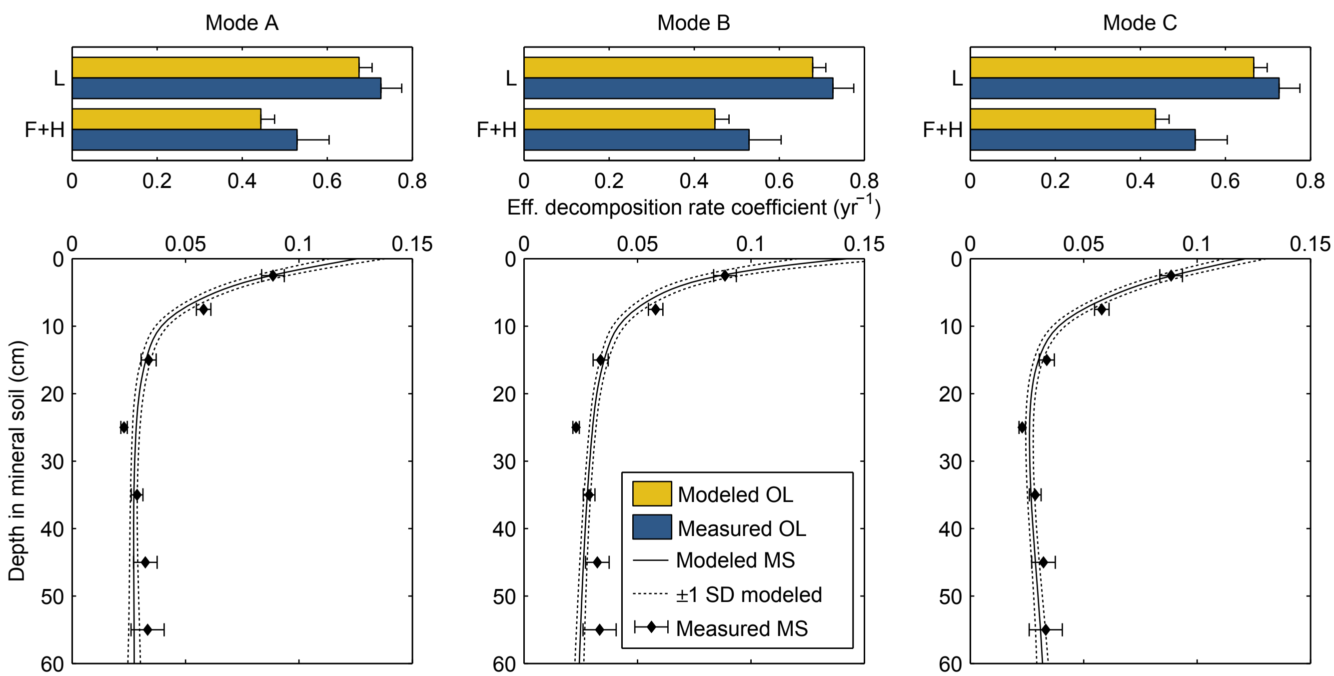

Figure 5: Measured effective decomposition rate coefficients and corresponding model results for Hainich, calibration setup 3. Depicted model results are averages and standard deviations over the Monte Carlo ensemble. Errorbars for the measurements indicate one standard error of the mean.

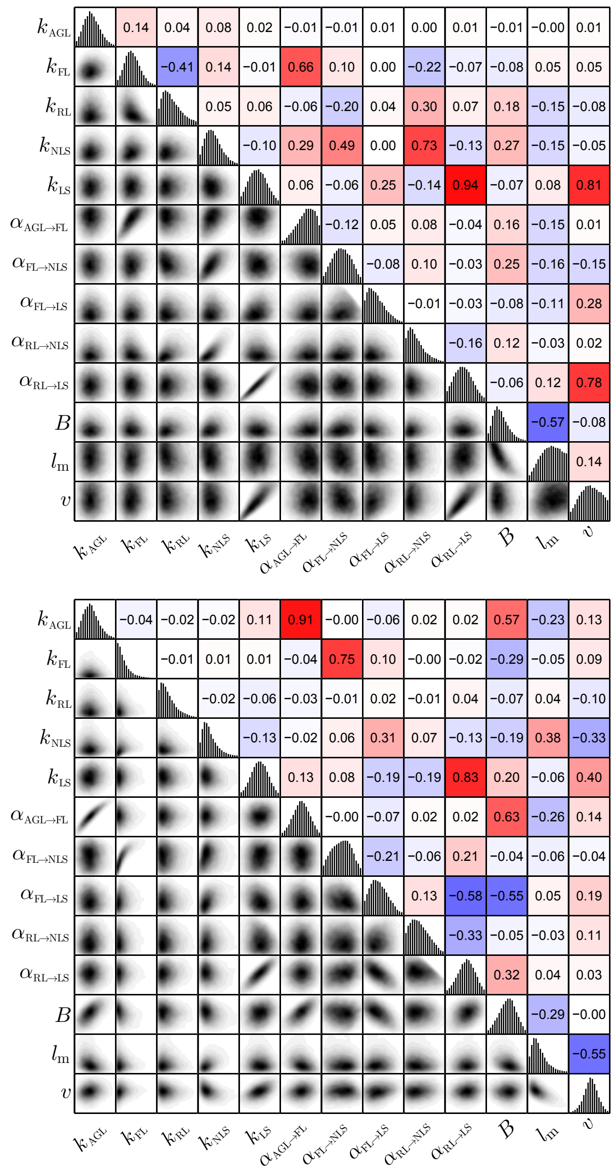

Figure 6: Correlation matrix of the posterior sample for calibration 3 (including $^{210}Pb_{ex}$ and strong priors) for Loobos and mode B for Hainich. The figures shows the correlations for each possible combination of two parameters. In the lower triangle bivariate density probability plots are depicted. In the upper triangle the correlation coefficients are shown, with blue indicating negative correlations and red positive correlations. On the diagonal histograms of the univariate marginal distribution for each parameter are shown.

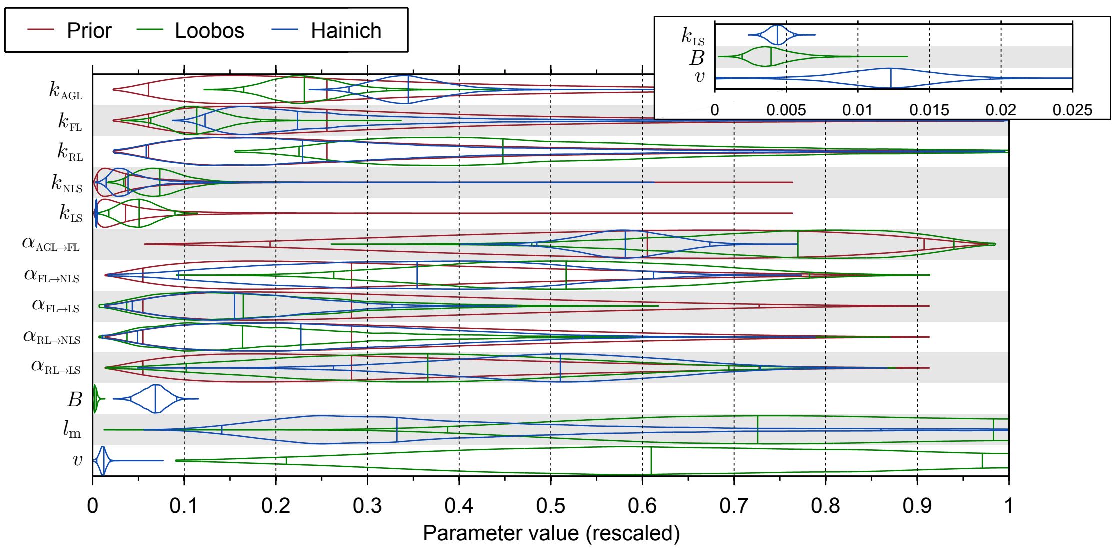

Figure 7: Marginal posterior distributions for Loobos and Hainich (mode B), calibration setup 3. The "violins" depict the marginal distribution for each parameter. The three vertical lines inside the violins indicate the median and the 95% confidence bounds.

Table 1: Observations used in the calibrations. Numbers are means and standard deviations of replicate samplings. Depth is relative to mineral soil surface. $^{210}Pb_{ex}$ fractions have been preprocessed and are relative to surface fraction (see section 2.3.2 in paper).

Description	**Depth (cm)**	**Mean**	**s.d.**	**N**
Loobos				
L horizon C stock ($kg\,C\,m^{-2}$)	n.a.	1.08	0.619	24
F horizon C stock ($kg\,C\,m^{-2}$)	n.a.	1.65	0.729	24
H horizon C stock ($kg\,C\,m^{-2}$)	n.a.	1.56	0.979	24
Mineral soil C stock ($kg\,C\,m^{-2}$)	2.07	0.417	21	
	0.5	1.11	0.312	21
Mineral soil C fraction (%)	3	0.550	0.153	21
	42.5	0.138	0.0413	21
Mineral soil $^{210}Pb_{ex}$ fraction (–), profile 1	1.25	0.623	-	1
	3.75	0.100	-	1
	6	0	-	1
	9	0.042	-	1
	13	0	-	1
Mineral soil $^{210}Pb_{ex}$ fraction (–), profile 2	1	0.614	-	1
	3	0.059	-	1
	5	0.028	-	1
	7	0	-	1
Hainich				
L horizon C stock ($kg\,C\,m^{-2}$)	n.a.	0.432	0.188	10
F/H horizon C stock ($kg\,C\,m^{-2}$)	n.a.	0.283	0.115	10
Mineral soil C stock ($kg\,C\,m^{-2}$)	n.a.	12.5	1.65	10
	2.5	6.63	1.50	9
	7.5	4.20	1.35	10
	15	2.400	0.0584	10
Mineral soil C fraction (%)	25	1.58	0.0196	10
	35	1.06	0.0253	10
	45	0.791	0.0337	10
	55	0.0597	0.0298	9
	65	0.0355	0.007	4
L horizon eff. decomp. rate coeff. (yr^{-1})	n.a.	0.685	0.0929	10
F/H horizon eff. decomp. rate coeff. (yr^{-1})	n.a.	0.459	0.0942	10
	2.5	0.0886	0.0150	10
	7.5	0.0580	0.00960	10
	15	0.0338	0.00992	10
Min. soil eff. decomp. rate coeff. (yr^{-1})	25	0.0229	0.00424	10
	35	0.0287	0.00774	10
	45	0.0323	0.0156	10
	55	0.0333	0.0206	9
	2.5	0.681	n.a.	1
	7.5	0.185	n.a.	1
	12.5	-0.0949	n.a.	1
Mineral soil $^{210}Pb_{ex}$ fraction (–)	17.5	0.0324	n.a.	1
	22.5	0.0776	n.a.	1
	27.5	0.0590	n.a.	1
	32.5	-0.0740	n.a.	1

Site	Mode	$\boldsymbol{k}_{\mathrm{AGL}}$	$\boldsymbol{k}_{\mathrm{FL}}$	$\boldsymbol{k}_{\mathrm{RL}}$	$\boldsymbol{k}_{\mathrm{NLS}}$	$\boldsymbol{k}_{\mathrm{LS}}$	$\boldsymbol{\alpha}_{\mathrm{AGL}\to\mathrm{FL}}$	$\boldsymbol{\alpha}_{\mathrm{FL}\to\mathrm{NLS}}$	$\boldsymbol{\alpha}_{\mathrm{FL}\to\mathrm{LS}}$	$\boldsymbol{\alpha}_{\mathrm{RL}\to\mathrm{NLS}}$	$\boldsymbol{\alpha}_{\mathrm{RL}\to\mathrm{LS}}$	$\boldsymbol{B}$	$\boldsymbol{l}_{\mathrm{m}}$	$\boldsymbol{v}$
		0.495	0.19	0.676	0.102	0.0531	0.479	0.263	0.0372	0.0376	0.102	0.00571	1.16	0.0211
Loobos	**n.a.**	0.735	0.297	1.68	0.184	0.189	0.658	0.5	0.171	0.148	0.487	0.00943	2.53	0.0651
		0.962	0.55	2.72	0.42	0.27	0.94	0.782	0.429	0.486	0.694	0.0232	2.95	0.0971
		0.873	0.3	0.212	0.00447	0.021	0.506	0.0276	0.0388	0.119	0.0424	0.185	1.3	0.0114
	A	1.08	0.381	0.598	0.00776	0.104	0.607	0.0845	0.149	0.309	0.162	0.256	1.86	0.0834
		1.45	0.484	2.35	0.0139	0.378	0.705	0.213	0.293	0.614	0.348	0.31	2.94	0.0978
		0.839	0.368	0.176	0.0444	0.00962	0.485	0.0939	0.0434	0.0491	0.263	0.125	0.423	0.000453
Hainich	**B**	1.1	0.746	0.788	0.0779	0.013	0.61	0.404	0.142	0.222	0.488	0.233	0.583	0.00137
		1.32	2.13	2.16	0.44	0.0165	0.674	0.612	0.327	0.535	0.729	0.276	2.58	0.00192
		1.01	0.318	0.018	0.0526	0.0306	0.582	0.0386	0.0283	0.0511	0.0795	0.247	2.24	0.0136
	C	1.21	0.439	0.0202	0.201	0.0389	0.647	0.247	0.0975	0.304	0.284	0.285	2.94	0.052
		1.76	1.1	0.0241	0.701	0.134	0.757	0.636	0.23	0.641	0.473	0.348	2.99	0.0972

Table 2: Properties of the marginal posterior distributions for both sites for calibration setup 3 (with $^{210}Pb_{ex}$ and strong priors). For each site/mode the 2.5 % quantile (upper), the sample with highest posterior density (middle), and the 97.5 % quantile (lower) are shown.