Implementation and initial calibration of carbon-13 soil organic matter decomposition in Yasso model

Jarmo Mäkelä[1], Laura Arppe[2], Hannu Fritze[3], Jussi Heinonsalo[4], Jari Liski[1], Markku Oinonen[2], Petra Straková[5], and Toni Viskari[1]

[1]Finnish Meteorological Institute, P.O. Box 503, FI-00101 Helsinki, Finland
[2]Finnish Museum of Natural History LUOMUS, P.O. Box 64, 00014, University of Helsinki, Helsinki, Finland
[3]Natural Resources Institute Finland, P.O. Box 18, FI-01301, Vantaa, Finland
[4]Department of Microbiology and Institute for atmospheric research INAR, Faculty of Agriculture and Forestry, P.O. Box 56, 00014 University of Helsinki, Helsinki, Finland
[5]Natural Resources Institute Finland, P.O. Box 2, 00791, Helsinki, Finland

Correspondence: Jarmo Mäkelä (jarmo.makela@fmi.fi)

Abstract. ~~Soil carbon sequestration has gained traction as a mean to mitigate rising atmospheric carbon dioxide concentrations. Verification of different methods' efficiency to increase soil carbon sink requires, in addition to good quality measurements, reliable models capable of simulating the effect of the sequestration practices~~Soils account for the largest share of carbon found in terrestrial ecosystems and their status is of considerable interest for the global carbon cycle budget and atmospheric carbon concentration. The decomposition of soil organic matter depends on environmental conditions and human activities, which raises the question of how permanent are these carbon storages under changing climate. One way to get insight ~~of the methods' effects on carbon cycling~~ into carbon decomposition processes is to analyse different carbon isotope concentrations in soil organic matter. In this paper we introduce a carbon-13 isotope specific soil organic matter decomposition add-on into the Yasso soil carbon model and assess its functionality. The new ^{13}C-dedicated decomposition is straightforward to implement and depends linearly on the default Yasso model parameters and the relative carbon isotope (^{13}C/^{12}C) concentration. ~~Despite of their simplicity, the~~The model modifications are based on the assumption that the heavier ^{13}C atoms are not as reactive as ^{12}C. The new formulations were calibrated using fractionated C, ^{13}C and δ^{13} measurements from litterbags containing pine needles and woody material, that were left to decompose in natural environment for four years. The introduced model modifications considerably improve the model behaviour in a ~~50-year long simulation~~100-year long simulation, where modelled δ^{13} is compared against fractionated peat column carbon content. The work presented here is a proof-of-concept and enables ^{13}C to be used as a natural tracer to detect changes in the underlying soil organic matter decomposition.

1 Introduction

~~Soil carbon (~~Earth system models (ESMs) are essential in our need to understand and examine the global carbon (C) ~~sequestration has been a serious topic of interest for several decades as a promising method to mitigate the rising atmospheric carbon dioxide (CO$_2$) concentrations. These type of methods aim to increase the soil carbon sink by~~ cycle, investigate the influence of environmental and human activities on it, and simulate possible future changes. One part of these complex models are

the land-surface components that, e.g.~~different soil tilling (?), crop rotation (?) or fertilisation practises (?). The fundamental problem related to C sequestration is how to demonstrate that the proposed management practice and land use change increase soil C stock size, and under what conditions and for how long the~~, describe the C ~~will remain in~~ stored in soils as well as the various interactions in soils and between vegetation and the ~~soil.~~

~~The quantification of small changes in soil C stocks is challenging due to large natural variability in soils and the large standing C stock. It has been estimated that the detection of 0.1 kg C m^{-2} change (approx. 1%) in an agricultural field in Finland where C stock size ranges between 8.4 and 9.8 kg m^{-2}~~ atmospheric boundary layer (?). Total C residing in soils has been estimated to be roughly 3000 Pg (?), but this estimate has large uncertainties as exact quantities are difficult to measure globally. Nevertheless, soils are the second largest global carbon pool, after oceans. The changing climate conditions are expected to influence the processes controlling C allocation into soils and the permanence of these storage pools (?). A simple approach to track changes in these processes and pools is to examine the ratio of carbon isotopes in, e.g., soil litter input and respiration. In order to fully utilise this approach, the underlying model must be capable of reliably simulating carbon-13 isotope (^{13}C) -related processes in the ~~top 30 cm requires hundreds of~~ soil~~samples to be analyzed (?). For this reason, an efficient verification system based on a combination of measurements (C stock size, CO$_2$ exchange, remote sensing etc.) and modelling is required and a new global vision of MRV (Monitoring, Reporting, Verification) platform was proposed by ?.~~

~~It is essential to understand which soil processes are the most important for soil~~C sequestration. The soil C pool can be divided into different fractions based on their chemical composition, physical characteristics or assumed turnover or residence times (?). Soil processes in general are complex as biological, chemical and physical drivers act simultaneously. For modelling purposes, the fate of ~~carbon-13 isotope (^{13}C) gives~~ can be used to test alternative model formulations and to give valuable additional information of the ~~parameter values of used model~~ optimal parameter values as the ^{13}C signatures are sensitive indicators of changes in processes. Soil organic matter (SOM) consists of molecules with different carbon isotopes. In theory, molecules with lighter ^{12}C atoms have lower activation (kinetic) energy requirements than those with ^{13}C. This leads to easier decomposition of ^{12}C-bearing compounds and enrichment of ^{13}C in residual organic molecules (?). ~~By estimating~~ Estimating ^{13}C in different fractions of SOM or varying residence times and adding ^{12}C/^{13}C reaction kinetics into the models would allow verification of the model functioning, and improve model predictions. ^{13}~~CO~~C-CO$_2$ measurements associated with gas flux measurements provide a promising way to link soil models to ecosystem models and allow further integration to ~~earth system models~~ ESMs, where ^{13}C isotopes are used to detect large scale C cycling patterns (?). Furthermore, the use of ^{13}C as a natural tracer enables more detailed examination of underlying C cycling processes (???).

~~There are a multitude of ways to improve MRV (?), but in our experience one method has not been as readily examined – that of carbon isotope composition~~ Additionally, soil carbon sequestration has been a serious topic of interest for several decades as a promising method to mitigate the rising atmospheric carbon dioxide (CO$_2$) concentrations. These type of methods aim to increase the soil carbon sink by, e.g., different soil tilling (?), crop rotation (?) or fertilisation practises (?). The fundamental problem related to C sequestration is how to demonstrate that the proposed management practice and land use change increase soil C stock size, and under what conditions and for how long the C will remain in the soil. The quantification of small changes in soil C stocks is challenging due to large natural variability in soils and the large standing C stock. It has been estimated that

the detection of 0.1 kg C m^{-2} change (approx. 1%) in an agricultural field in Finland where C stock size ranges between 8.4 and 9.8 kg m^{-2} in the top 30 cm requires hundreds of soil samples to be analyzed (?). For this reason, an efficient verification system based on a combination of measurements (C stock size, CO_2 exchange, remote sensing etc.) and modelling is required

60 and a new global vision of MRV (Monitoring, Reporting, Verification) platform was proposed by ?. An overlooked approach to improve MRV is to examine the C isotope compositions in the soil and in heterotrophic respiration. The reason behind the lack of ~~such~~ these examinations is simple, such approaches require a model that can reliably represent the soil organic carbon (SOC) dynamics for different carbon isotopes while still retaining relatively straightforward structure. The latter is especially important when we take into account the lack of good-quality calibration and validation data.

65 In this paper we introduce a simple ^{13}C isotopic circulation into the recently re-calibrated SOC model Yasso ~~(???)~~(???). In our approach, the decomposition of ^{13}C-specific soil organic matter (^{13}C-SOM) is linearly dependent on the default Yasso model parameters, the carbon isotope fraction ^{13}C/^{12}C and a new scaling factor θ, that represents change to the decomposition rate between the carbon isotopes. The underlying hypothesis behind this design is that since ^{13}C has a larger atomic weight it is therefore not as reactive as ^{12}C, but environmental factors should still affect the decomposition of SOM, containing either

70 isotope, similarly. We calibrate the new ^{13}C-related decomposition parameters (θ) and assess the model functionality both on short and long term (~~50-year~~ 100-year simulation) basis.

Our aim is to improve Yasso20 model parameterisation ~~(?)~~ (?) to include ^{13}C/^{12}C reaction kinetics in the model by using empirically measured SOM and ^{13}C data. ~~We~~ The purpose of this paper is to provide a proof-of-concept and we hypothesize that measuring ^{13}C in soil organic matter fractions 1) detects differences in the pool ^{13}C content supporting the ^{13}C-fractionation and enrichment theory, and 2) allows model development for ~~significant~~ future improvements in SOM decomposition predic-

75 tions as ^{13}C can be used as a tracer to detect changes in the underlying C decomposition processes.

2 Materials and methods

2.1 Measurements

The SOC measurements were derived from experiments described in ???, where different types of plant litter was left to
80 decompose inside litterbags in natural environment at Lakkasuo, a raised bog complex in Central Finland (61.8°N, 24.3°E, 150 m.a.s.l.). We utilised data detailing the conditions for pine branch and pine needle specific litterbags. In addition to determining the initial states for both litter types, 14 litterbags describe the soil conditions for pine branches and seven for pine needles at later stages of decomposition during the four-year-long experiment.

The litter was characterized by dividing it into carbon fractions by sequential extractions and hydrolysis according to Hi-
85 lasvuori et al. 2013 (and references therein), also called AWEN extraction (acid, water, ethanol, non-soluble). In short, this included analysing the amounts of nonpolar extracts (corresponds to E), polar extracts (W), acid hydrolysable substances (A) and non-soluble Klason type substances (N). Air dried litter material was ground in a mill (Fritsch) to pass the 0.5 mm sieve and weighted into a centrifuge tube (35 ml). The amount of extractables was determined through the remaining mass after shaking (2h or 18h; 250 rpm) with the different solvents followed by filtering through glass crucibles (Robu, Borosilicat 3.3

por. 4). At the start of the extraction procedure 0.5 g litter mass was used. Dichloromethane (CH_2Cl_2; 15 ml; repeated twice) was first used to remove the nonpolar extractives. 0.35 g of the remaining dried (105 °C) solid sample was weighted again into a centrifuge tube and hot water (80 °C; 15 ml) was added and kept in a water bath (80 °C; 18 h). After centrifugation ($1500 \times g$) the pellet was washed with 30 ml hot water to finish the extraction for polar extractives. In all cases the respective extractives were combined and dried. Evaporation was used for the nonpolar fraction and warming (50 °C) followed by freeze drying was polar fraction. 0.1 g oven dried (105 °C) material from the residue left after the hot water extraction was weighted into a centrifugation tube and 1.25 ml 72% sulphuric acid (H_2SO_4) was added and shaken in room temperature (1 h; 250 rpm). Thereafter 35 ml water was added and incubated in a water bath (95 °C; 18h) followed by filtration. The remaining mass (Klason lignin) was washed once with hot water (95 °C; 30–40 ml) and the mass was dried o/n in 105 °C. Each fraction ie. the original litter, the solid remains after dichloromethane, water and acid extraction and from the evaporated nonpolar and polar extractants, subsamples were analysed for their relative $^{13}C/^{12}C$ ratios as $\delta^{13}C$ values. The definition of $\delta^{13}C$ is given below, where $\left(\frac{^{13}C}{^{12}C}\right)_{standard} = 0.01123720$ is the Vienna Pee Dee Belemnite (**?**, VPDB).

$$\delta^{13}C = \left(\frac{\left(\frac{^{13}C}{^{12}C}\right)_{sample}}{\left(\frac{^{13}C}{^{12}C}\right)_{standard}} - 1 \right) \cdot 1000‰. \tag{1}$$

The isotopic composition of carbon was measured on a NC2500 elemental analyzer coupled to a Thermo Scientific Delta V Plus isotope ratio mass spectrometer at the Laboratory of Chronology, Finnish Museum of Natural History. The raw isotope data were normalised with a multi-point calibration using certified isotopic reference materials (USGS-40, USGS-41, IAEA-CH3 and IAEA-CH7). The mean measured (pre-normalization) $\delta^{13}C$ values for calibration references were -26.52 for USGS-40, +36.19 for USGS-41, -24.88 for IAEA-CH3, and -32.27 for IAEA-CH7, with an r^2 of > 0.999 between measured and expected values. Replicate analyses of quality control reference materials analysed alongside the unknowns indicate a 1σ internal precision of ≤ 0.20. For the purpose of model calibration, all samples were scaled to represent the same amount of original matter (we use 1000 mass units of original matter – the given C and ^{13}C values are in relation to this value).

In addition to litterbag measurements, we have utilised peat profile measurements, detailed in **?**, to examine long-term carbon decomposition with the Yasso model. The corresponding profile is given in Table 1 and the age of the three top-most layers is based on radiocarbon signatures (**?**), which could not be used to accurately estimate the other two layers. We have naively set their age to 20-years each. The fractionated $\delta^{13}C$ content of these layers is taken directly from Table 2 in (**?**) and their relation to the Yasso fractions will be given in the results.

The meteorological variables required to run the Yasso model were extracted from a nearby weather station measurements (**?**), located at Hyytiälä (61.85°N, 24.29°E, 180 m.a.s.l.). We gathered monthly temperature and annual precipitation from the beginning of year 2005 to the end of 2008. Additionally we calculated averaged monthly temperature and averaged annual precipitation from years 2000–2014 to be used in simulating the long-term carbon decomposition.

2.2 Yasso model

depth	layer age
0–20 cm	0–30 years
20–26 cm	30–40 years
26–32 cm	40–50 years
32–38 cm	50–70 years
38–44 cm	70–90 years

Table 1. Peat profile used to examine long-term carbon decomposition.

The soil carbon model Yasso was originally built to simulate the soil carbon stock and changes in this stock for forest soils (**?**). Previous versions of the Yasso model have also been incorporated into land-surface models, see e.g. **?** for Yasso implementation to JSBACH – the land-surface component of the Max Planck Institutes Earth System Model (MPI-ESM). We generate the soil carbon pools utilising ~~the Yasso SOC model (?). The underlying model version is the~~ a recently re-calibrated version of the
125 model called Yasso20 ~~(?) with parameter values given~~ (**?**). This calibration utilised multiple global datasets and we present relevant model parameter values in appendix Table A1. We ~~have introduced~~ introduce a new ^{13}C specific decomposition into this model, which utilises new parameters (θ, explained below). When all $\theta \equiv 0$, both ^{12}C and ^{13}C use the same standard decomposition parameters, hence we call this model the default Yasso model and the new version, with optimised θ parameters, as Yasso-C13 or optimised Yasso, when we need to make a distinction. Otherwise both models are simply referred to as the
130 Yasso model.

Yasso decomposes litter into different pools that represent acid, water and ethanol (A, W and E) soluble matter and a lignin-like pool (N), all the pools having different decomposition rates. The decomposed C is released back to the atmosphere as heterotrophic respiration, shifted between the AWEN pools or transferred to inactive humus (H) pool. The model is driven with monthly temperature and annual precipitation. The SOC pool decomposition in the Yasso model can be represented by
135 the following equation.

$$x_t = Mx_{t-1} + b_t \tag{2}$$

The state vector (x_t), representing the C content in AWENH pools at time t, is calculated by operating the state transition matrix (M) on the state vector of the previous time step (x_{t-1}) and adding litter input (b_t), which in our simulations is set to zero (as we assume no litter is added into the litterbags after the beginning). The model initial state (in our simulations) is set
140 to match the first measurements. The matrix ~~M determines the decomposition of SOM and the flow of carbon between the different pools and it is dependent on various parameters as well as temperature and precipitation.~~ $M = FK$ is a product of fluxes (F) between the pools and decomposition (K). Pool-specific decomposition rates ($k_i, i \in$ {A,W,E,N,H}), presented in Eq. 3, are dependent on certain parameters (θ, γ, β), base decomposition rates (α_i), and functions depicting the effect of woody

145
$$k_i(\theta) = \frac{\alpha_i}{J} h(d) \left(1 - e^{\gamma_i P}\right) \sum_{j=1}^{J} e^{\beta_{i,1} T_j + \beta_{i,2} T_j^2} \tag{3}$$

We introduce ^{13}C-SOM decomposition into the Yasso model by adding separate ^{13}C-specific storages for each AWENH pool and including an additional ^{13}C-specific SOM decomposition step. The input data (essentially carbon content) is first separated into ^{13}C-specific content and the rest ~~, which we call ^{12}C although it also contains ^{14}C~~ of the carbon. The Yasso model is first run normally ~~with ^{12}C~~ as in Eq. 2, which is followed by ^{13}C decomposition using a modified version of the ~~state~~

150   ~~transition matrix M. We modified the diagonal elements of M (these determine the SOM decomposition within each pool) by replacing the parameter (α) affecting the diagonal element with:~~ pool-specific base decomposition rate:

$$\alpha_i^\star = \left(1 + \frac{^{13}\text{C}}{^{12}\text{C}}\theta\right)\alpha_i. \tag{4}$$

~~Essentially, we include~~

The new coefficients $\alpha_i^\star$ replace α_i in Eq. (3), which essentially introduces a dependency for the mass ratio of the carbon
155   isotopes (^{13}C/^{12}C) as well as a free parameter θ ~~for each AWEN~~ to the Yasso model for each ^{13}C-AWEN pool separately. We didn't include a parameter for the humus pool (H) as we did not have measurements to calibrate the related parameter. ~~We also note here that the diagonal elements are further dependent on temperature and precipitation, but these model aspects were not modified. Further details on Yasso model can be found in ?~~ Additionally, we do not include the humus pool in the bulk carbon examinations for the same reason – bulk carbon refers to the total sum of carbon in AWEN pools.

160   ## 2.3   Model calibration

We calibrated the four θ parameters related to the decomposition of each AWEN pool ^{13}C-SOM. The objective function (f) of the calibration is the cumulative squared error of the observed and modelled δ^{13}C values:

$$f = \sum_i (\delta^{13}\text{C}_{i,\text{modelled}} - \delta^{13}\text{C}_{i,\text{observed}})^2. \tag{5}$$

Here the summation is taken over all AWEN pools and available litterbag measurements (with measurements indicating zero
165   concentration for total carbon content removed from the calculations). The unnormalised (pointwise) parameter likelihood is calculated as $\mathcal{L} = e^{-f}$.

Since we had only four parameters to calibrate, we ~~set similar initial limits for the parameters and a suitable increment that determined how densely the parameter values were distributed~~ produced a parameter grid by fixing an increment and giving each parameter a initial value of zero. Then we added multiple new values symmetrically around the initial value with the
170   given increment. We ran the model with every member of the parameter "grid" to get an estimate of the overall shape of the parameter likelihood ~~and to test for reasonable limiting values for the parameters~~. This process was repeated several times with ~~refocused grid and readjusted increment.~~

~~Presented are marginal likelihoods for each calibrated parameter as well as likelihood dependencies between each two parameters, calculated by setting the other parameters to their optimal values.~~ grid re-centered to the point with maximum

175 likelihood and with readjusted (smaller) increment. The results were also verified with independent runs using different initial values. All experiments were run on a 8-core laptop utilising RStudio version 1.4.1103. We used the R interface of Yasso (see code and data availability) in addition to R.utils version 2.10.1 (no other libraries were needed).

3 Results

The Yasso model calibration resulted in strictly unimodal parameter probability distributions (Fig. 1). This was not unexpected

180 as each calibrated parameter could only directly affect a single AWEN pool. The optimised parameter values are $\theta_A = -0.289$, $\theta_W = -0.205$, $\theta_E = -0.004$ and $\theta_N = 0.055$ (we also note that the precision of the calibration was left at the third decimal as likelihood values started to plateau). ~~The elongated shape of the likelihood dependencies between two parameters indicate some correlation between the parameters (Fig. 1).~~ When we examine the parameter combinations with highest likelihoods (top 250 values), the strongest correlations (≈ 0.77) are present between θ_A and θ_W, θ_A and θ_N as well as θ_W and θ_N.
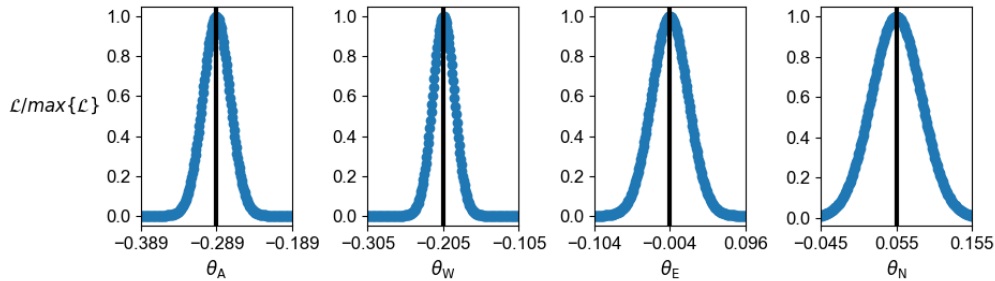

Figure 1. ~~Shown~~ Presented are ~~timeseries produced by~~ the ~~default and optimised Yasso model versions for~~ pointwise parameter likelihoods (when setting the ~~different AWEN pools together with assimilated observations~~ other parameters at their optimal values), divided by the maximum likelihood value. The ~~model results for C and ^{13}C concentrations are on top of each other~~ vertical lines indicate the parameter value with the highest likelihood.

185 The default and optimised parameter values were used to generate SOM decomposition and related C, ^{13}C and δ^{13}C time-series from the given initial states (Fig. 2). The differences between the simulated ^{13}C concentrations are too small to be evident (C concentrations are identical), but we get a clear signal from the δ^{13}C values. ~~Overall, both~~ The default model depicts changing δ^{13}C, which is driven by differences in the initial isotopic fractions between the pools and the rate of the flow of carbon between the pools.

190 Both model versions tend to underestimate the speed of SOM decomposition (the C and ^{13}C concentrations) at Lakkasuo ~~for~~ (Fig. 2) for the A and N pools and overestimate for the W pool. The bulk carbon content behaves similarly to A and N pools as these contain the most carbon. The default Yasso model is reducing the relative ^{13}C content (reducing the δ^{13}C values) for the
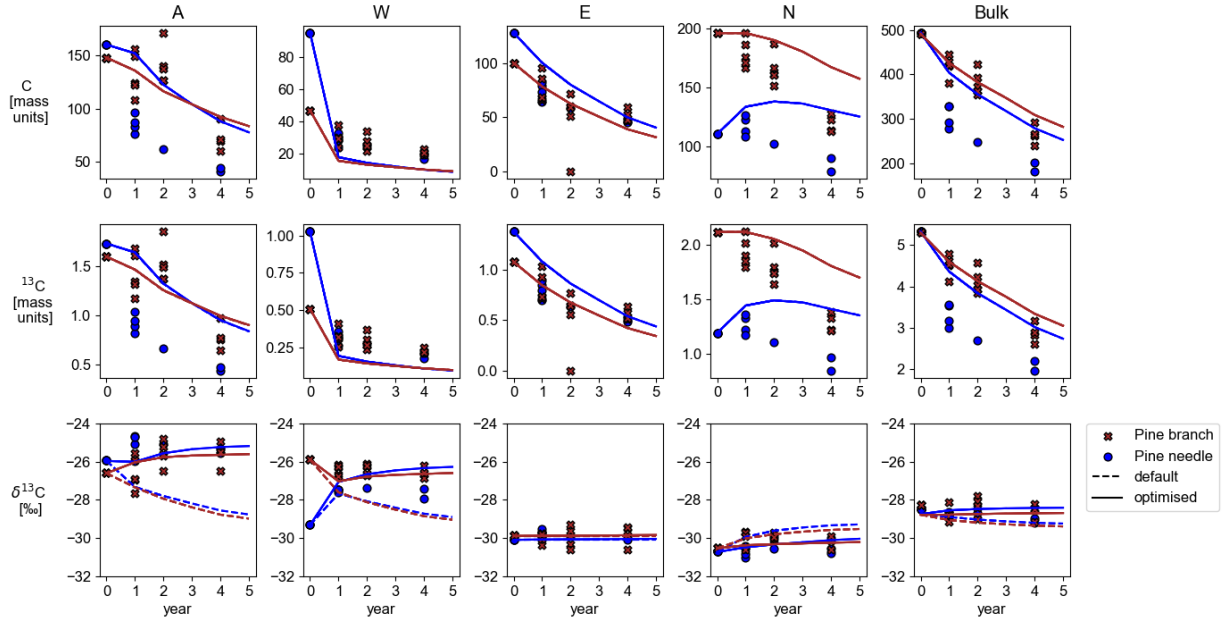
Figure 2. Shown are timeseries produced by the default and optimised Yasso model versions for the different AWEN pools together with assimilated observations. The model results for C and ^{13}C concentrations are on top of each other.

A and W pools and deviating from the observations whereas the optimised model version seems to be increasing the relative ^{13}C content and following the observations more closely. There is no apparent difference for the E pool, but the calibration has lowered the rate of ^{13}C enrichment for the N pool. We have calculated and gathered the mean and standard deviation of the corresponding pointwise δ^{13}C model bias values (model - observations) for the individual AWEN pools to Table 2.

Table 2. Calculated default and optimised model bias (model - observations) mean and standard deviation for the different AWEN pools.

	A-δ^{13}C		W-δ^{13}C		E-δ^{13}C		N-δ^{13}C		Bulk-δ^{13}C	
	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ
default	-2.2	1.05	-1.29	0.74	-0.07	0.36	0.47	0.49	-0.49	0.44
optimised	-0.102	0.76	-0.003	0.63	-0.04	0.37	-0.08	0.4	-0.02	0.44

The Lakkasuo initial states and generated average year (averaged monthly temperature and annual precipitation) from years 2000–2014 were used to simulate a ~~50-year~~ 100-year long carbon decomposition (Fig. 3). This simulation can be compared to Lakkasuo peat column δ^{13}C values at different depths ~~(?, Table 2) that we have naively equated to the simulation at regular 10-year intervals~~ given in Table 1 and in ?. The holocellulose values are comparable to the A pool, Klason to the N pool,

8

nonpolar extracts to the E pool and polar extracts to the W pool. A noteworthy detail is that on short term (Fig. 2) the default model increased the relative ^{13}C content (δ^{13}C values) of E and N more than the optimised version, but on longer timescale this situation is reversed ~~for E and projected to reverse for N~~ (Fig. 3). The difference in δ^{13}C values for bulk C, between the default and optimised model versions at the end of the 100-year long simulation, translates to approximately 0.3‰ difference in C mass percentage.
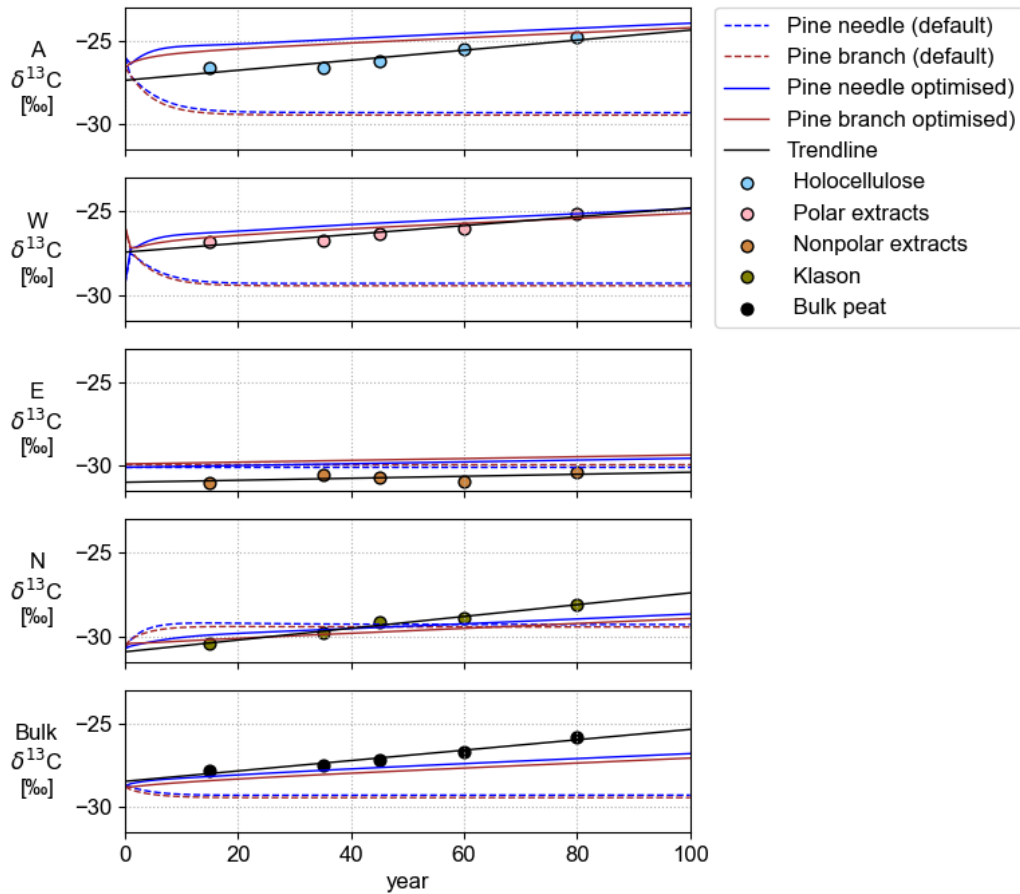
Figure 3. Timeseries of simulated δ^{13}C values of the different AWEN pools for the default and optimised Yasso model versions. Scatter-plotted are peat column ~~composition~~ δ^{13}C values ~~(?, Table 2)~~ at different depths, positioned at the midpoint of assumed age, along with corresponding trendlines.

4 Discussion

We have introduced simple modifications to the Yasso model in order to account for ^{13}C-SOM decomposition. Incorporation of δ^{13}C on SOM decomposition models is a necessary step towards integration of Earth system and dynamic land ecosystem models. The δ^{13}C values of different organic compounds or chemical fractions of mixed organic material can be used as natural
210 tracers which provide a unique tool to investigate and uncover complex decomposition processes in ~~soil.~~ the soil. Examples of such approaches include, e.g., examination of tree carbon use by chasing ^{13}C-CO$_2$ pulse in the respiration of leaves, whole crowns, roots, and soil (**?**); an analysis of how stable isotope fractionation might be used to identify microbial function without incubation in soil samples (**?**); and assessment of carbon uptake and respiration fluxes *via* the use of ^{1}3C depleted CO$_2$ (**?**).

In the current study, we introduced new θ parameters to account for ^{13}C-SOM decomposition in the Yasso model. The
215 calibration of these parameters only depend on the δ^{13}C values, i.e. the relative carbon isotope concentrations, and revealed unimodal distributions for all four AWEN pool related parameters. Considering the acquired optima and taking into account that generally the ratio ^{13}C/^{12}C ≈ 0.01, then the new ^{13}C-SOM decomposition utilises values that differ at maximum 3‰ (for θ_A) from the default decomposition parameter values. Therefore, it is not surprising that both default and optimised model versions generate nearly identical SOM decomposition both on a short (Fig. 2) and long term~~(we did not provide this image~~
220 ~~as it provides no additional value)~~. Moreover, the 0.3‰ relative difference in bulk C between the model versions at the end of the 100-year simulation is too small to be used directly to improve bulk C estimates. The benefits come in the various ways ^{13}C can be used as a natural tracer.

The acquired optima for θ_A, θ_E and θ_W are all negative, which ~~in the model~~is consistent with the initial hypothesis and ^{13}C-fractionation and enrichment theory. In the model, this translates to reduced ^{13}C-SOM decomposition rate (Fig. 2). Like-
225 wise, the positive value for θ_N implies increased ^{13}C-SOM decomposition when compared to the default model. However, the reduction in δ^{13}C values, when compared to the default model version, is only true on shorter timescales (Fig. 2) as each pool has a ~~clear~~ trend to increase relative ^{13}C content during the ~~50-year~~ 100-year long simulation (Fig. 3). This is due to the reduced ^{13}C-SOM decomposition in other pools – as there is more ^{13}C present in these pools, there is more ^{13}C available to be transported into the N pool, which compensates for the increased decomposition. ~~This situation is not ideal, but understandable~~
230 ~~as Yasso also operates in the terms of "bulk" soil – there are no soil layers or~~ The positive θ_N goes against the initial hypothesis, but is a direct result of model structure. It could be worthwhile to investigate how modifications to the model, such as adding multiple soil layers with differences in the effects of temperature, precipitation or Q10 ~~at different soil depths~~ (see e.g. Fig. 1 in **?**), would improve the model capabilities.

The straightforward changes to the Yasso model have improved the model capabilities in reproducing observed δ^{13}C values
235 in short (Fig. 2) and longer timescales (Fig. 3). Results from the ~~50-year~~ 100-year long simulation seem to corroborate the initial hypothesis for A,W and N pools that the relative ^{13}C content in soil (larger δ^{13}C values) increases with time. The optimised model even yields a positive trend for E pool δ^{13}C whereas the default model tends to converge the δ^{13}C values of all pools to roughly -30. The ~~peat decomposition at different depths (?, Table 2) can be naively approximated to be of different~~ ~~ages at 10-year intervals. The~~ optimised model behaviour follows the trend of these measurements and the results are highly

240 encouraging, even though the model is driven with a single averaged year representing the meteorological conditions from the beginning of the 21st century.

As estimation and modelling of soil organic matter decomposition, but also C sequestration, are current scientific challenges~~, our modified model demonstrates how measurable delta-13 values can be used to improve SOM decomposition model~~. We have demonstrated how ^{13}C can be implemented into a soil carbon model, so that carbon isotope signals could then be used

245 to analyse carbon cycles in more detail and to improve model capabilities, accuracy and predictability. The required model modifications were straightforward and resulted in drastic improvement of modelled δ^{13}C values of SOM extracts. Although we emphasize the preliminary nature of our results due to limited calibration dataset, we foresee the model to act as a truly important tool to understand the role of isotopic fingerprints within soil carbon decomposition. The ~~Yasso-C13 model should be tested and parameters evaluated using~~ experiments demonstrated here should be viewed as a proof-of-concept, but further

250 research is needed to verify the model capabilities on other sites, ecosystems and larger areas. Future research is expected to also include different management practices and croplands. Since the production of AWEN extractions with δ^{13}C measurements is labour-intensive, future research will likely rely on inverse calibration on larger δ^{13}C datasets that are rather straightforward to produce, or meta-analysis using literature-based values could be also used for further evaluation across varying scales (local, regional, global).

5 Conclusions

255

We have demonstrated how to incorporate ^{13}C-SOM decomposition into the Yasso model and calibrate it. The model modifications were simple and straightforward and resulted in ~~greatly~~ significantly improved simulated δ^{13}C values. The results support the initial hypothesis of ^{13}C-fractionation and enrichment theory. The capability of a model to simulate soil ^{13}C content and ~~to better simulate~~ isotope-specific SOM decomposition improves the applicability of Yasso-C13 model to scale process from

260 ecosystem level to regional and global using δ^{13}C as a tracer. Conceptually the presented work is on solid ground, but the lack of suitable calibration and validation data urges further studies ~~that produce~~ with new, precise experimental δ^{13}C data suitable for Yasso-C13 model calibration and validation. ~~Likewise further efforts should be made to include soil layers into the Yasso model.~~

11

Appendix A: Yasso model parameters

Table A1. Utilised Yasso model parameter values.

Description	Parameter	Value
Base decomposition rate for A pool	α_A	0.51
Base decomposition rate for W pool	α_W	5.19
Base decomposition rate for E pool	α_E	0.13
Base decomposition rate for N pool	α_N	0.1
Mass transfer fraction from W to A	p_{WA}	0.5
Mass transfer fraction from E to A	p_{EA}	0
Mass transfer fraction from N to A	p_{NA}	1.0
Mass transfer fraction from A to W	p_{AW}	1.0
Mass transfer fraction from E to W	p_{EW}	0.99
Mass transfer fraction from N to W	p_{NW}	0
Mass transfer fraction from A to E	p_{AE}	0
Mass transfer fraction from W to E	p_{WE}	0
Mass transfer fraction from N to E	p_{NE}	0
Mass transfer fraction from A to N	p_{AN}	0
Mass transfer fraction from W to N	p_{WN}	0.163
Mass transfer fraction from E to N	p_{EN}	0
First order temperature impact parameter for AWE	a_{AWE}	0.158
Second order temperature impact parameter for AWE	b_{AWE}	-2.0×10^{-3}
First order temperature impact parameter for N	a_N	0.17
Second order temperature impact parameter for N	b_N	-5.0×10^{-3}
First order temperature impact parameter for H	a_H	0.067
Second order temperature impact parameter for H	b_H	0
Precipitation impact parameter for AWE	g	-1.44
Precipitation impact parameter for N	g_N	-2.0