~~The impact of c~~Calibrating~~ng~~ the soil organic carbon model Yasso20 with multiple datasets

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Abstract. Soil Organic Carbon (SOC) models are important tools ~~in determining~~for assessing global SOC distributions and how carbon stocks are affected by climate change. Their performances are, however, affected by data and methods used to calibrate them. Here we study how the Yasso SOC model performs if calibrated individually or with multiple datasets and how the chosen calibration method affected the parameter estimation. We found that when calibrated with multiple datasets, the model showed a better global performance compared to a single dataset calibration. Furthermore, our results show that more advanced calibration algorithms should be used for SOC models due to ~~the~~ multiple local maximas in the likelihood space.

1. **Introduction**

Soils are the second largest global carbon pool, hence even small changes in this pool impact the global carbon cycle (Peng et al. 2008). However, Soil Organic Carbon (SOC) and associated~~SOC~~ changes are difficult and laborious to measure (Mäkipää et al., 2008). They can also vary drastically over space due to differences in litter fall, site and soil type as well as climate (Jandl et al., 2014, Mayer et al., 2020). Hence, ~~Soil Organic Carbon (~~SOC~~)~~ models are important tools for~~in~~ estimating current global soil carbon stocks and their future development (Manzoni and Porporato, 2009). ~~Soils are the second largest global carbon pool, hence even small changes in this pool impact the global carbon cycle (Peng et al. 2008). However, SOC and SOC changes are difficult and laborious to measure (Mäkipää et al., 2008). They can also vary drastically over space due to differences in litter fall, site and soil type as well as climate (Jandl et al., 2014, Mayer et al., 2020). Hence, to quantify the global SOC stocks and estimate the effects of different drivers, such as changing environmental conditions, on SOC stocks (Sulman et al., 2018, Wiesmeier et al, 2019), numerous~~ Numerous SOC models have been developed in the past decades (Parton et al., 1996; Cammino-Serrano et al., 2018; Thum et al., 2019) to quantify the global SOC stocks and estimate the effects of different drivers, such as changing environmental conditions, on SOC stocks (Sulman et al., 2018, Wiesmeier et al, 2019).

While majority of SOC models rely on linear equations representing the movement of C within the soil, there has been studies showing the need to ~~Three central research challenges have emerged in the development of SOC models. First, the majority of such models still rely on linear equations representing the movement of C within the soil. This approach has been questioned by the arguments that~~ represent at least some of the SOC processes such as the microbial influence ~~or response to a large scale environmental change need to be~~

~~represented~~ by non-linear equations (Zaehle et al., 2014; Liang et al. 2017) or that the state structure of the model affects which kind of data can be used to calibrate it (Tang and Riley, 2020). More complicated SOC models addressing these arguments have been developed, for example Millennial (Abramoff et al, 2018), and modules including additional drivers affecting the C pools have been included in existing SOC models, such as nitrogen (Zaehle and Friend, 2010) and phosphorus (Davies et al, 2016; Goll et al., 2017) cycles. Their implementation is hindered, though, by that~~e second challenge as~~ detailed data is~~are~~ needed to constrain the model parameterization, but individual measurements campaign datasets are often limited in size and lacking in ~~detail~~ nuance of the SOC state (Wutzlerand and Reichstein, 2007; Palosuo et al., 2012). Consequently, multiple datasets representing different processes should be used to parameterize the models in order to capture the multitude of SOC dynamics, but combining observation datasets with varying spatial scales, measurement temporal densities, inherent assumptions and structural errors can cause issues with adequately incorporating all the information (Oberpriller et al., 2021). The chosen calibration methodology is additionally affected by the same issues based on its approach of fitting the data. ~~this naturally raises questions on combining different datasets, and impact of choice of calibration methodology on the resulting parameter sets. Third, decomposition rate dependence on SOC compounds, spatial variation in SOC stocks and different drivers and environmental conditions pose challenges to SOC model calibration.~~

~~While there are measurements that can constrain certain processes, there is no single measurement set that reliably captures all the elements.~~ Litterbag decomposition experiments (Harmon et al., 2009) provide information on the faster decomposition processes, but their applicability to longer-term assessments have been questioned (Moore et al., 2017). Furthermore, even in current studies it is common to use only data from one litterbag decomposition experiment campaign (for example Kyker-Snowman, 2020) due to the differences in experimental setups and physical properties of the litterbags making direct comparison of results difficult. Organic carbon content can be measured from soil samples, but those measurements provide a limited snapshot because of the large number of measurements needed to detect changes and the slow dynamics of SOC (Mayer et al. 2020). Additionally, the SOC in these measurements cannot effectively be fractionated into different state components used in the models. Hence, assumptions need to be made on the amount of short-lived SOC to approximate the amount of long-lived SOC. There are also other aspects of litter that are known to affect the decomposition rate, e.g. the bigger the size of the woody litter the slower the decomposition is (Harmon et al., 2000), which requires detailed and specific observations to inform models.

The Yasso07 model (Tuomi et al., 2009) was developed to address some of these challenges. In it, both the litter inputs and the soil carbon are divided into chemically measurable fractions that decompose at their own rate which are affected by environmental conditions, specifically ambient temperature and moisture. This direct link between the model state and litter input allowed using different litter decomposition experiment data to constrain model parameters. One of the core ideas in the development of Yasso07 is the parameterization process itself is done simultaneously with multiple datasets reflecting different parts of the SOC decomposition process in a Bayesian calibration framework (Zobitz et al., 2011). As a part of this approach, litterbag specific leaching term was introduced in order to be able to use information from several litterbag experiments at the same time (2011b).

While the initial Yasso07 calibration addressed the challenges regarding the variety of data required, it did not touch in detail on the issues affecting the actual SOC model parameterization process. First, the Yasso07 did not calibrate all the parameters simultaneously with all the data, but instead calibrated the parameters in segments where the previously calibrated parameters were set as constant when calibrating the next set of parameters (Tuomi et al., 2011). While this makes the calibration process easier, it naturally also affects the results and associated uncertainties as well. Second, there has been no standard methods established to evaluate how the inclusion of additional datasets impacts the general performance of SOC models. In other words, does using multiple datasets improve the model estimates? Naturally, this applies to Yasso07 as well. Third, there have been studies which indicate that the choice of parameterization method does matter in ecosystem modelling (Lu et al., 2017). It is reasonable to assume that would also hold true for SOC systems where there could be multiple parameter sets that can potentially produce a local fit into the data. Last, but not least, the previous Yasso07 calibration workflow was not easily repeatable and reproducible to allow inclusion of new datasets and algorithms.

In this study, we built~~d~~ upon previous Yasso developments ~~and~~ to present a ~~new~~ model formulation that expanded on how the environmental drivers affect the decomposition. The data used to calibrate the model is the same for both versions with the exception of the measurement data regarding long-term carbon allocation. For Yasso07, a time series dataset from Southern Finland while for Yasso20, approximated steady state SOC measurements from across the world was used to constrain the relevant parameters. Additionally, we use a more advanced model calibration method in association with a stricter protocol on what kind of data points were used for calibration and an open source R package for data inclusion, repetition and reproduction of calibration.~~ and a calibration protocol,~~ The model and produced parameter set ~~that we~~ will refer to as~~call~~ Yasso20 hereinafter. Our redesigned calibration protocol leverages BayesianTools R-package (Hartig et al., 2019), an open source general-purpose tool for Bayesian model calibration. Using BayesianTools in our workflow, we ~~not only~~ not only established a more reproducible and standardized application of Yasso20 calibration, but also leveraged interfacing with multiple calibration algorithms and examined the role of the calibration method.

Due to the nature of the available SOC related datasets we hypothesize: I) the SOC model performs better globally if multiple datasets are simultaneously used to constrain it compared to a SOC model calibrated with an individual dataset despite the numerous assumptions required for combining the different information, II) the likelihood space created by these multiple datasets is uneven with multiple maxima to the degree that more advanced parameter methods are necessary for the end result not to be dependent on the starting point, and that III) These changes in the model formulation and the calibration protocol will improve how the Yasso model projections performance compared to the previous model version.~~Due to the nature of the available SOC related datasets we hypothesize: I) the SOC model performs better globally if multiple datasets are simultaneously used to constrain SOC models compared to a SOC model calibrated with an individual dataset despite the numerous assumptions required for combining the different information, and that II) the likelihood space created by these multiple datasets is uneven with multiple maxima to the degree that more advanced parameter methods are necessary for the end result not to be dependent on the starting point. advanced parameter estimation methods~~

~~account better for multiple potential likelihood maximas than simpler methods, and II) the SOC model performs better globally if multiple datasets are simultaneously used to constrain SOC models compared to a SOC model calibrated with an individual dataset.~~

~~The first hypothesis is tested by comparing the Yasso parameter values produced by parameter estimation methods of varying complexity and how well they converge. Second~~ The first hypothesis is tested by calibrating the Yasso with individual datasets as well as the combined data sets with the resulting performances compared using numerous validation datasets. All these calibrations are done for all the parameters simultaneously. The secondt hypothesis is tested by comparing the Yasso parameter values produced by parameter estimation methods of varying complexity and how well they converge. Furthermore, the more extensive calibration process has allowed constraining more details in the new Yasso formulation which is introduced here as well.

2. Methods

2.1 Yasso model description

The Yasso model is based on four basic assumptions on litter decomposition and soil carbon cycle: 1) Litter consists of four groups of organic compounds (sugars, celluloses, wax-like compounds and lignin-like compounds) that decompose at their own rate independent of origin (Berg et al., 1982). 2) Decomposition of any group results either in formation of carbon dioxide (CO_2) or another compound group (Oades, 1988). 3) The decomposition rate is affected by environment temperature and moisture (Olson, 1963; Meentemeyer et al., 1978; Liski et al., 2003). 4) The diameter size of woody litter determines the decomposition rate (Swift, 1977). Yasso20 is the next version of Yasso (Liski et al. 2005) and Yasso07 models (Tuomi et al., 2009, 2011b) and continues to build on these same assumptions. The main formulation contribution in Yasso20 compared to the previous versions is the added nuance in how climate drivers affect the different pools, which in turn is possible here due to the improved calibration scheme. For the purposes of the calibration here, another assumption was necessary: 5) The most stable soil carbon compounds are only formed in the soil as a result of bonding with mineral surfaces (Stevenson, 1982). The following model formulations apply for Yasso20.

Based on the previously established assumptions, litter can be divided into four fractions according to their chemical composition. Compounds soluble in a polar solvent (water) represent sugars (W) and those soluble in a non-polar solvent (ethanol or dichloromethane) represent wax-like compounds (E). Compounds hydrolyzable in acid (for example sulphuric acid) represent celluloses (A) and the non-soluble and non-hydrolyzable residue represents lignin-like compounds (N). Additionally, there is a fifth compartment, humus (H), which represents long-lived, stable soil organic carbon produced by interaction with mineral compounds in the soil. As the carbon compounds are broken down by the decomposition processes, they become either new compounds belonging to another compartment or CO_2. The decomposition rate of each compartment is considered independent of the litter origin and affected by a temperature, moisture, and size component.

The masses (x) of the compartments at time t are denoted by vector $x(t) = [x_A(t), x_W(t), x_E(t), x_N(t), x_H(t)]$. The Yasso model uses an annual timestep and determines the changes in those masses according to

$$\frac{\partial x(t)}{\partial t} = M(\theta,c)x(t)^T + b(t), \quad (1)$$

where *b(t)* is the litter input to the soil at the time *t*, *θ* is the set of parameters driving decomposition as defined in Table 1 and *c* contains the factors controlling the decomposition. As not only are accurate soil moisture estimates challenging to obtain for the measurements used here, but a vast majority of them are from the surface. Thus, air temperature *T* and precipitation *P* were used as the environmental drivers along with the woody litter diameter *d*. Operator **M** is the product of the decomposition, as presented by K, and mass fluxes between compartments, as depicted by F, equations as follows

$$M(\theta,c) = F(\theta)K(\theta,c),$$

(2)

$$F(\theta) = \begin{bmatrix} -1 & p_{WA} & p_{EA} & p_{NA} & 0 \\ p_{AW} & -1 & p_{EW} & p_{NW} & 0 \\ p_{AE} & p_{WE} & -1 & p_{NE} & 0 \\ p_{AN} & p_{WN} & p_{EN} & -1 & 0 \\ p_H & p_H & p_H & p_H & -1 \end{bmatrix}, \quad (3)$$

$$K(\theta,c) = diag, \quad (4)$$

Here parameters $p_{ij} \in [0,1]$ denote the flows from compartment *i* (*i* ∈{A,W,E,N}) to *j* (j∈{A,W,E,N,H}) and are included in the parameter vector *θ*. The decomposition rates $k_i(\theta,c)$ were calculated according to

$$k_i(\theta,c) = \frac{\alpha_i}{J}h(d)(1-e^{\gamma_i P})\sum_{j=1}^{J} e^{\beta_{i1}T_j+\beta_{i2}T_j^2}, \quad (5)$$

where the base decomposition rate α_i, temperature parameters β_{i1},β_{i2}, and precipitation parameter γ_i for compartments $i \in \{A,W,E,N,H\}$ are all a part of the parameter set *θ*. The temperature and precipitation dependent rate parameters are the same for compartments AWE, but both N and H compartments are given their own separate parameter values. In order to capture the annual temperature cycle more efficiently, the average monthly temperatures for all 12 months are given as an input with the model averaging over their impacts as seen in eq. (5). The total annual precipitation is used instead of monthly precipitation as seasonal variation such as snowfall or heavy rainfall followed by long dry stretches would hinder the calibration if the monthly precipitation was used. The temperature and precipitation equations are established in Tuomi et al. (2008). Woody litter decomposition rate in response to diameter (*d*) is described in *h(d)* based on Tuomi et al. (2011), as follows,

$$h(d) = min((1+\varphi_1 d+\varphi_2 d^2)^r, 1), \quad (6)$$

where φ_1, φ_2, and *r* are parameters included in the parameter set *θ.*

Given initial state x_0, average environmental conditions *c* and constant litter input *b(t)* = *b*, the model prediction can be computed by solving the differential equation in Eq. (1). The solution becomes

$$x(t) = M(\theta,c)^{-1}\left(e^{M(\theta,c)t}(M(\theta,c)x_0+b)-b\right), \quad (7)$$

where the matrix exponential is determined numerically. In a steady state situation $x = \lim_{t\to\infty} x(t)$, equation 7 becomes

$$x = -M(\theta, c)^{-1} b, \qquad (8)$$

2.1.1 Yasso20 improvements

Two main changes were introduced to the Yasso20 version here compared to the earlier Yasso07 version. The first change was that the temperature input for Yasso20 is given as the mean monthly temperature for each month of the year instead of the mean annual temperature and associated annual temperature amplitude. This was done in order to better represent the more nuanced global temperature profiles. For example, the previous scheme was indifferent if the winter was long or short, which is, however, expected to affect the annual decomposition. The second change was to differentiate the climate driver impacts between the AWE, N and H pools instead of using the same parameter values for all the model C pools. This was done because previous research established that more complex carbon compounds require more energy to be broken up (Davidson and Janssen, 2006), which indicates that the parameters representing those dynamics should also differ between pools. It is expected that these changes will affect the model performance and the calibration results themselves, especially as this allows the environmental conditions to impact the pools differently. Thus this changed model version was decided to be a new version of the model. We do not compare Yasso20 performance to Yasso07 here. All model parameters given in Table 1 were targeted in the calibration.

2.2 Datasets used in the calibration

Several datasets were simultaneously used to calibrate the model in order represent different processes related to soil carbon cycling: Decomposition bag time series data from the Canadian Intersite Decomposition Experiment (CIDET; Trofymov, 1998), Long-Term Intersite Decomposition Experiment (LIDET; Gholz et al, 2000) and European Intersite Decomposition Experiment (ED; Berg et al., 1991a, 1991b) projects, a collection of global soil organic carbon measurement gathered by Oak Ridge National Laboratory (Zinke et al., 1986) and woody matter decomposition dataset from Mäkinen et al. (2006). In addition to these large datasets, a smaller litter bag decomposition data set from Hobbie et al. (2005) was used to both evaluate how much addition of a comparatively small number of data points affects the calibration results as well as an independent validation dataset for the other calibration parameters. These datasets along with additional details are listed in Table 2.

CIDET, LIDET and ED are litter bag decomposition timeseries where litter is left to decompose in a mesh bag and the remaining mass is measured at chosen time intervals over several years. Each dataset had the experiments with multiple different species, with the initial chemical composition also provided by the dataset, and different sites. Furthermore, while CIDET and LIDET only measured the remaining mass, ED also determines the AWEN fraction from one of the replicant samples, which allows us to directly compare it to the Yasso20 state variables. However, while in CIDET and LIDET the remaining mass has ash removed, in ED ash is still included in the remaining mass. The mean monthly temperatures and precipitations have been measured at each test site with the annual precipitation being summed up from the monthly precipitation values.

The global SOC measurement dataset from Oak Ridge National Laboratory (Zinke et al., 1986) is collected from the data of numerous unrelated projects that have measured SOC as a part of their campaign. As such, there are/were no uniform applicable protocols to these measurements. For the purposes of the calibration, the data is assumed to represent the steady state SOC at that location and each measurement is treated as independent from the others even if they are from the same location. Furthermore, we only used SOC measurements that were below 20 kgC m^{-2} in the calibration. Values higher than those were found in high latitudes and considered as results of waterlogging, peat formation or permafrost, processes not described in Yasso20. The litter input was determined by combining the global GPP map from Beer et al. (2010) with the global NPP/GPP relationship set to 0.5 at the measurement locations due to lack of specific information on the NPP/GPP there. The Olson classification (Olson et al., 2001) regarding the local ecosystem type was used to roughly divide the ecosystems into grasslands, semi-forests and forests. The litter fractioning for these different systems are given in Supplemental Table 1. In addition, SOC chronosequence data from Liski et al. (1998) and plot level measurements of Liski and Westman (1995) was used as a validation data set.

The woody decomposition data used here is from Mäkinen et al. (2006), which has measurements of multiple trees in different stages of decomposition over several decades in Finland. There are no signifiers to connect the measurements from different years nor to indicate how much the tree diameter has been reduced over time because the data was not chronosequence data of the same trees. As such, the measurements were considered independent and representative of decomposition of a tree trunk of that size.

The same litterbag and woody data were used to calibrate both Yasso07 and Yasso20. The sole exception regarding the litterbag data is that the whole ED dataset was used in Yasso07 calibration while in Yasso20 we removed decomposition data from manipulation experiments. However, Yasso07 H pool parameters were not parameterized with the Oak Ridge data. Instead, the chronosequence data from Liski et al. (1998) was used in its calibration with climate and litterfall drivers derived from Southern Finland conditions (Tuomi et al., 2009). As already established, this dataset was not used in Yasso20 calibration and was only applied as a validation dataset.

2.2.1 Dataset uncertainties

The information of the uncertainty related to the measurements was limited. With CIDET and LIDET there are generally four replicants, sometimes less, from which the standard deviation in remaining mass can be calculated. Similar standard deviation is available for the ED measurements, but is only determined for the total mass loss and not for the AWEN pool measurements used here. Furthermore, there are other aspects affecting the uncertainties such as the ED measurements containing ash or LIDET measurement time series showing more noise than the CIDET measurements. For the global SOC dataset and the woody matter decomposition datasets no such replicant deviation is available nor is there any other established uncertainty. There are other similar measurement campaigns where uncertainty estimates are given, but it is not clear how directly they can be applied for the datasets used here. Consequently, here we used our expert opinion to determine the different dataset uncertainties relative to each other (Table 1) as we felt this was a more transparent manner to acknowledge the current limitations regarding assigning the uncertainties.

Systematic differences in the litter bag properties affected the use of different datasets (Tuomi 2009; Tuomi2011b). In general, high mass loss rates were positively correlated with a large mesh size of the litter bags and high precipitation in our datasets. This is because the decomposing material in the litter bags is partially 'washed away' into the surrounding soil by water flow and is thus removed from the bag due to processes other than decomposing. To correct for this, we added a leaching term to equation 1 as follows,

$$\frac{dx(t)}{dt} = (A(\theta, c) - \omega_{site} P I_5)x(t) + b(t), \quad (9)$$

where ω_{site} is the dataset-specific leaching term and $\mathbf{I}_5$ is a 5×5 identity matrix. This approach was simplified as there are multiple components expected to affect the leaching process and other systematic errors, but it was necessary to establish even this simplistic initial approach for the work here.

Finally, long-lived carbon compounds represented by the H pool in the Yasso model are not produced in decomposition litter bags as they require organo-mineral associations which are unlikely to occur in the litter layer"

that is only possible in the soil. Because of this p_H (transfer fraction from AWEN pools to pool H) could have non-zero values only with the Oak Ridge global SOC dataset.

2.3 Calibration protocol

We used the BayesianTools R-Package (Hartig et al., 2019) in our calibration workflow for its standardized and flexible implementation of Markov chain Monte Carlo (MCMC) algorithms with external models, as well as for its post-MCMC diagnostic functionality. While our main aim in this paper was not to compare MCMC algorithms, once the interface was established with the BayesianTools, it was trivial to leverage the common setup and test the performances of different MCMC flavors as implemented by the package. We found this exercise helpful as our calibration problem involves a relatively high dimensional and irregular likelihood surface. It has been previously shown that for such systems the efficacy of the calibration may differ between algorithms (Lu et al., 2017). Thus, we tested two robust and efficient algorithms Differential Evolution Markov Chain with snooker updater (DEzs, ter Braak and Vrugt, 2008) and Differential Evolution Adaptive Metropolis algorithm with snooker updater (DREAMzs, Vrugt et al., 2009; Laloy and Vrugt, 2012; Vrugt, 2016), in addition to the long-established adaptive Metropolis (AM) algorithm (Haario et al., 2001).

All three algorithms use Markov chains to explore the parameter space and generate samples from the posterior. However, AM uses a single chain, whereas DEzs and DREAMzs use multiple interacting chains simultaneously. While DREAM emerged from DE, DREAM further uses adaptive subspace sampling to accelerate convergence

(Vrugt, 2016). All three algorithms use proposal distributions to generate successive candidate samples and grow the chains. However, AM uses a multivariate Gaussian distribution as the proposal which is most effective when the target distribution (a.k.a. posterior) is also Gaussian. Whereas, DEzs and DREAMzs algorithms use the differential evolution principle to optimize the multivariate proposals (with snooker jumps to increase the diversity of the proposals), automatically adjust the scale and orientation of the proposal distribution according to the target distribution (Vrugt et al., 2009; 2016). As a result of these properties, especially when not tuned properly, AM can take much longer to complete the high-dimensional parameter search and can suffer from premature convergence when multiple distant local optima are present (Vrugt, 2016; Lu et al., 2017). Whereas DEzs and DREAMzs can potentially resolve non-gaussian, high-dimensional and multimodal target distributions more effectively without much configuration (Laloy and Vrugt, 2012, Lu et al., 2017).

In our calibration protocol, we ran 3 chains for each algorithm where DEzs and DREAMzs further tripled each chain. We initialized these chains from the prior distributions (Table 1) using the random sample generator of the BayesianTools package. Each chain was run for 1.5 x 10^6 iterations and the last 1.5 x 10^5 iterations were used to compute the posterior probability distributions after removing the burnin. Convergence diagnostics were checked by visually inspecting the trace plots of the chains, as well as calculating the multivariate R-statistic of Gelman and Rubin (1992).

For the likelihood function we used a simple approach where the uncertainties are assumed to be normally distributed and independent of each other. In the litterbag experiments because the absolute uncertainty remains the same over time while the amount of decomposing litter decreases, the relative uncertainty increases over time. There are uncertainty dynamics affecting the data in reality that is not accounted for here such as more nuanced time dependence of the uncertainties, uncertainty auto-correlation in a time series and non-normally distributed uncertainties. Due to not having reliable information to properly assess how these effects should be included into the likelihood calculations here, we chose the described basic approach. This is considered to make it more straight-forward to later add the missing uncertainty dynamics as approximations of them become available and examine how those inclusions affect the calibration results.

Initially the calibration was done with all the parameters associated with the Yasso20 model. However, if the estimated parameter values for the p-terms in eq. 3 were within three decimals from either 0 or 1, they were set to nearest limit value of 0 or 1, after which the calibration was redone. During the calibration, the p value parameterization can never settle at 0 or 1 and, hence, it is impossible to know what the real p value is that close to the limit. The calibration results presented here only had four p values that were not set: p_{WA}, p_{WN}, p_{EW} and p_{EA}. Parameters p_{AW} and p_{NA} were set to 1 and the other AWEN related p values were set to 0. Furthermore, since we assumed that only decomposition in the W pool results in CO2, we estimated only p_{EW} and set p_{EA} to be the E-pool remnant from 1 with p_{EN} set to 0.

2.4 Validation protocol

Each of the litter decomposition experiments (CIDET, LIDET and ED) was randomly split into two: data used for calibration (80% of the measurements) and data used for validation (20% of the measurements). Furthermore, the random division is done so that the whole measurement time series from one bag is always fully either in calibration or validation data. It was also verified that each site and species in was approximately equally represented in both the calibration and the validation data. Due to the noise and bias in both the global SOC measurement data sets in addition to the separate processes included in those calibrations, we did not divide them into calibration/validation parts but used all the data for calibration.

The experiments were conducted by calibrating the Yasso model individually with the calibration data from each litter bag decomposition data set (CIDET-only, LIDET-only, ED-only) as well as a joint calibration that used all the calibration data detailed before (i.e. CIDET, LIDET, ED, Mäkinen, global SOC). The leaching parameter was individually calibrated for each decomposition bag dataset during the joint calibration. In addition, the Hobbie3 dataset (Hobbie, 2005) was used as an independent validation dataset. Since there was no information on its leaching parameter, that was set to zero in the validation runs. The validation for each calibration results was done with all the separate validation data sets. Similar validation dataset is created with the Mäkinen wood decomposition data with 20 % of the data points set aside for validation purposes. There was, however, no independent calibration done with the Mäkinen dataset as there is not enough of data there to constrain the model completely and in the validation analysis the focus was on how it performed over wood size instead of time.

The global Oak Ridge SOC data set was not split into calibration/validation parts for two reasons. First, as it was the only dataset calibrating the H parameters, there was no efficient to way to evaluate how the addition of new data would have impacted the model performance regarding this dataset. Second, the dataset was found to be so noisy that the randomized choosing of the validation datapoints already affected the results to a noticeable degree. Due to this, the H parameter calibration was evaluated with two separate small datasets. First, SOC measurements from several plots Hyytiälä, Finland (Liski & Westman, 1995) where the dominant tree species of each plot is known was used to test if Yasso20 was able to calculate an approximately correct SOC value for the plots. The SOC values for plots with the same dominant species were averaged for the comparison with the litterfall used for each species listed in Supplemental Table 2. Second, a SOC chronosequence from Liski (1998) was used to determine if Yasso20 is able to realistically simulate the SOC accumulation over time scales of hundreds of years. In this dataset there are 26 soil age gradient data points from the Finnish coast which has been used to approximate the SOC accumulation in the soil over hundreds of years after the ice age. Tree litter and climate driver data from Hyytiälä, Finland was used here as the main focus is on if the simulated system reaches steady state in the same time window as the measurements. The climate driver data used for these validation runs is included in Supplemental Table 3.

2.5 Yasso07/Yass020 comparison protocol

During the calibration of Yasso07, there was no separate validation data set aside for the CIDET, LIDET and ED and all the data was used for the parameterization. Because of that we do not use those validation datasets for the model performance comparison. Instead, only the Hobbie3 validation dataset and the Hyytiala plots are used for to determine if there is any notable improvement in Yasso20 performance with them compared to

Yasso07. For the litterbag data, the comparison shall be the RMSE while for the Hyytiala plots how the model projected steady state SOCs compare to the measured plot values.

To assess the differences in the model over long-term decomposition, both models were used to model the decomposition of a hypothetical straw litter (A=620 g, W=50 g, E=20 g, N=310 g) over a 100-year time period with the Hyytiälä, Finland climate drivers. This is not based on any measurement time series and is purely a synthetic test.

3. Results

3.1 Calibration performance

The first step was to determine if there is a notable difference in how the different calibration methods perform with the global dataset. All three calibration methods (AM, DEzs, DREAMzs) produced similar maximum a posteriori (MAP) values for global (joint) calibration where all data streams were used (Figure 1, Supplemental Table 4~~3~~). Closer examination of different chains~~ (Figure 1)~~, though, shows that while DEzs and DREAMzs converged to the same parameters, individual AM chains instead produced different parameter distributions. Closer examination of different chains, though, shows that while DEzs and DREAMzs converged to the same parameters, individual AM chains instead produced different parameter distributions and thus the calibration itself did not converge. The AM chain parameter distributions already settled into these distributions based on the initial parameter values given to them and even after doubling the number of iterations (Not shown) the distributions remained the same. In our view, this is indicative of what would happen if a simple single chain calibration was done with SOC models. The Gelman-Rubin (G-R) statistics for the different calibration methods (Supplemental Table ~~3~~4) reflect these differences in convergence as well, with DEzs having the values within the acceptable boundary while values for AM are above acceptable ranges. DREAMzs also performs generally well but shows more divergence with the parameter values than DEzs. Similar behaviour was seen when running the individual dataset calibrations, where individual AM chains would mix well, but converged at different values from each other (Not shown). Per global calibration diagnostics of different algorithms, we decided to report the rest of the results with the DEzs algorithm for clarity as its estimates were converging best out of the three examined methods. When the global calibration with the DEzs algorithm was repeated with the Hobbie3 data set included, the resulting parameter distributions were nearly identical to the calibration done without the Hobbie3 data set included (Not shown).

3.2 Parameter estimates and correlations

The next step was to examine how the use of multiple datasets simultaneously affected the calibrated parameter sets compared to when using only individual datasets for calibration. ~~When comparing calibrations done with the DEzs approach for the individual data sets as well as the global calibration that used all that data (Figure 2; Table 4), t~~The parameter sets produced by the calibrations differ from each other to a meaningful degree in both the parameter mean value as well as the associated uncertainty range (Figure 2; supplemental table 5). Despite that, though, there are certain patterns in the parameter sets: The pool decomposition rate relationships remain the same in that W has the quickest turnover rate followed by A with N being the slowest to decompose. With the climate terms, both CIDET and LIDET calibrations have difficulties in settling on the climate terms while covering multitude of different climate types while ED calibration, where the climate differences between measurement locations are minor, produces a relative narrow climate parameter estimate. The global calibration, however, does clearly converge around certain climate parameters even if the uncertainty range is remains wide. And even though the ED dataset has the most detail about the AWEN distribution, the AEW decomposition rates estimated based on it do not appear to converge with multiple peaks in the parameter distributions.

To further examine the parameter calibration, we ~~A~~analyzed~~ing~~ the correlations between different parameter values produced by the DEzs algorithm from the global calibration (Figure 3~~7~~), which shows that the correlations are the strongest between processes affecting the same pools. The p-terms which had been set to 0 and 1 were excluded from the correlation analysis since they did not vary during the calibration. The AWE pools decomposition rates have strong positive correlations between the decomposition rates as well as with the climate driver terms affecting decomposition in them. Similarly, there are strong negative correlations between the temperature terms affecting the same pools and a strong positive correlation between the H pool terms. There are both strong positive and negative correlations with the size related parameters. While the exact correlation values changed depending on the calibration dataset, the general relationships remained similar (Not shown).

3.3 Validation and comparison to Yasso07

The final step was to validate how the different parameter sets perform with separate validation datasets and determine if there are notable systematic errors with regard to the climate driver data. For each dataset, the RMSE values are at their lowest when using the parameter sets calibrated with that specific dataset (Table 3~~5~~), though the global parameter set produced RMSE values close to those lowest values. However, when using the parameter sets calibrated by other datasets than the validation data have been chosen from, the RMSE values became higher indicating worse model performance. When the RMSE analysis was done with the Hobbie3 dataset, the global parameter showed the best performance. It should be noted that since in the ED data set measurements are for each individual AWEN pool, the individual measurements are smaller in value than the total mass measurements of CIDET/LIDET/HOB3. Consequently, the RMSE values for ED are smaller than those for CIDET/LIDET/HOB3 datasets.

With regard to the long-term SOC projections, the comparisons with the Hyytiälä forest plot measurements (Table 4~~6~~; Figure 4~~3~~) indicates that at least in the Nordic forests Yasso20 potentially slightly overestimates the steady state SOC, with the largest differences still being below 2 kg C m^{-2}. It should be noted, though, that there is notable variance within the measurements in addition to the uncertainty related to the driver data. The chronosequence data (Figure 5~~4~~) shows that the model projection saturates approximately in 1000 years similarly to the measurements.

When examining how Yasso20 performs relative to Yasso07, the RMSE for Yasso07 projections is 118.2 grams compared to the Yasso20 RMSE of 110 grams. With the Hyytiälä forest plot measurements (Table 4), in all plots Yasso07 overestimated the SOC by at least 3 kg C m^{-2} more than Yasso20. However, when examining the distribution of carbon into different pools in these steady states (Not shown), more meaningful differences were revealed. For Yasso07, only ~37 % of the SOC was in the long-lived H pool while ~50 % of the carbon was in the N pool. By comparison, with Yasso20 projections ~54 % of the carbon is in the long-lived H pool and ~27 % in the N pool.

The hypothetical straw litter decomposition (Figure 6) shows that while the total carbon remainder for the two models are close to each other for the first 10 years, after that there is a clear divergence between the model projections with Yasso07 having higher remaining carbon than Yasso20. More detailed inspection of the results (Not shown) found that this difference was due to the N pool decomposing at a much slower rate than in Yasso07 than in Yasso20. This also causes less carbon to accumulate in the H pool in Yasso07 than in Yasso20 with the latter having approximately twice as much carbon in the H pool than the former after 50 years. When repeated with warmer climate drivers (Not shown), Yasso07 time series projection decreases at a faster rate than Yasso20 time series projection.

3.4~~2~~ Residual analysis

When checking residuals from the litter bag experiments against mean annual temperature, annual temperature variation and total annual precipitation (Figure 7~~65~~), there appears to be a tendency for Yasso20 to increasingly underestimate the remaining litter bag C with growing average mean temperature and precipitation. The error does not, though, show any signal when looking at the temperature variation within the year. With the woody decomposition residuals (Figure 8~~76~~), there is a slight negative trend over time and a slight positive trend over size. Both are minor, though, and the residuals for the woody decomposition are relatively evenly distributed for the validation dataset.

~~3.3 Parameter values correlation~~

~~Analyzing the correlations between different parameter values produced by the DEzs algorithm (Figure 7) shows that the correlations are the strongest between processes affecting the same pools. The p-terms which had been set to 0 and 1 were excluded from the correlation analysis since they did not vary during the calibration. The AWE pools decomposition rates have strong positive correlations between the decomposition rates as well as with the climate driver terms affecting decomposition in them. Similarly, there are strong negative correlations between the temperature terms affecting the same pools and a strong positive correlation between the H pool terms. There are both strong positive and negative correlations with the size related parameters.~~

4. Discussion

The benefit of calibrating with multiple datasets

Our results show that simultaneously using multiple datasets from different environments improves the general applicability of the SOC model even when having to use the simplistic leaching factor approach to be able to compare different litter bag datasets and lacking detailed uncertainty estimates, confirming our first hypothesis. This is in line with prior studies arguing for larger representation in the calibration data (Zhang et al., 2020). Furthermore, a more detailed analysis of different calibrations shows (Figure 2) indicates that the information from multiple datasets is in truth even necessary for the calibration as when calibrating only with one dataset, the decomposition parameter uncertainty ranges either were large or, in the case of the more nuanced EuroDeco dataset, don't even appear to converge.

Further inclusion of smaller dataset

Even with this global calibration, individual locations can be affected by specific SOC decomposition conditions not currently accounted for in the models (Malhotra et al., 2019). Naturally, if smaller datasets of SOC and decomposition measurements are available from locations affected by specific decomposition dynamics, for example agricultural soils that are treated in a very specific manner, it would be logical to use that local information to constrain the SOC model to better suit that location. However, the results here raise questions on how those smaller datasets should be implemented in the model calibration. The inclusion of the Hobbie3 dataset did not meaningfully impact the calibration results (Not shown), which is reasonable considering how small that litterbag dataset (N=192) is compared to the totality of the other datasets (N=~17 000 of which $N_{litterbag}$ = ~12 000) being used in the calibration. This indicates that due to the sheer size of the global calibration data set, smaller local data sets cannot effectively be used just by adding it to the joint calibration process. Additionally, while the smaller datasets such as the Hobbie3 datasets contain site specific information, they are similar measurements as the ones within CIDET and LIDET and, thus, there is no reason to believe they would provide additional insight to the global application. There are other options, though, by either using the globally estimated parameter ranges as the priors for a calibration with the local data, re-weighing the different datasets based on expert opinion (Oberpriller et al., 2021) or employing a hierarchical calibration approach (Tian et al., 2020, Fer et al., 2021), but the impact of these approaches should be separately researched and tested. Our study still successfully provided a global parameter set that increases the applicability of Yasso model and informs global SOC estimates.

Calibration method

Here we showed that by using a DEzs calibration algorithm, we were able to simultaneously use multiple different types of datasets to constrain the soil organic carbon (SOC) model Yasso and produce a converging parameter set. Additionally, using a more conventional model calibration approach, here the Adaptive Metropolis (AM), showed that it was vulnerable to the local likelihood maximas and that the resulting parameter sets were strongly affected by the starting values. This supports our ~~first~~ second hypothesis that more advanced calibration methods ~~should be used~~ are necessary to better explore the likelihood surface and estimate SOC model parameters due to the ~~numerous local likelihood maximas~~trade-offs between the parameter values that result in equifinality in the parameter space~~, especially when detailed algorithm configurations are not always possible or desirable~~. Furthermore, even the more stable calibration method produced different results for different individual datasets used to calibrate. ~~The global calibration set, in turn, proved to be most efficient~~

~~across different datasets, indicating that multiple datasets should be used to constrain SOC models.~~ More advanced calibration methods, though, then need to be applied to minimize the impact of the resulting uneven parameter space and producing Gelman-Rubin values within more acceptable ranges (Gelman and Rubin, 1992). Something that was curious in our results was that DEzs converged better than DREAMzs (Supplemental Table ~~3~~4) despite the latter being a more state-of-the-art method (Vrugt, 2016). We were not able to determine the reason for this in our tests here, specifically was it something related to the behaviour of the parameter space or to some aspect of the technical implementation~~how the method is implemented in BayesianTools~~.

Impact of prior parameter information

One of the fundamental challenges for calibrating SOC models is lack of experimental information regarding the model parameter value distributions. Therefore, we used generally broad uniform prior distributions for the calibration here. However, it is still important to evaluate the calibration results based on our understanding of the overall system behaviour. For example, initially we used wider priors for parameters p_H and α_H (Results not shown), which in turn resulted in the calibration producing a p_H value of ~0.08 and, consequently, a much higher H pool decomposition rate. As this did not fit with the system behavior seen i.e. with the bare fallow experiments (Menichetti et al., 2019) or the soil chronosequence (Fig 3-3), we applied a narrower prior constraint on the related parameters. Another, and a more, complicated example is that when using wider prior constraints for the N pool decomposition rate parameter α_N, the calibration resulted in the N pool being largely insensitive to the temperature and moisture drivers. While there are no direct measurements of the lignin pool temperature sensitivity, there have been studies showing that the energy needed for breaking down SOC compounds increased with complexity (Davidson and Janssen, 2006; Karhu et al., 2010) indicating that the N pool should be temperature sensitive. Here we chose to constrain α_N to a lower range, which in turn forced a climate driver sensitivity for it. All these examples illustrate that prior information and expert opinion should directly inform the calibration and the calibration results themselves should further be reassessed in their physical meaning.~~All these examples illustrate that the calibration results themselves should further be reassessed in their physical meaning.~~

~~The benefit of calibrating with multiple datasets and further inclusion of smaller datasets~~

~~Our results show that simultaneously using multiple datasets from different environments improves the general applicability of the SOC model confirming our second hypothesis. This is in line with prior studies arguing for larger representation in the calibration data (Zhang et al., 2020). However, even with this global calibration, individual locations can be affected by specific SOC decomposition conditions not currently accounted for in the models (Malhotra et al., 2019). Naturally, if smaller datasets of SOC and decomposition measurements are available from locations affected by specific decomposition dynamics, for example agricultural soils that are treated in a very specific manner, it would be logical to use that local information to constrain the SOC model to better suit that location. However, the results here raise questions on how those smaller datasets should be implemented in the model calibration. The inclusion of the Hobbie3 dataset did not meaningfully impact the calibration results (Not shown), which is reasonable considering how small that dataset (N=192) is compared to~~

~~the totality of the other datasets (N=~17 000) being used in the calibration. This indicates that due to the sheer size of the global calibration data set, smaller local data sets cannot effectively be used just by adding it to the joint calibration process. There are other options, though, by either using the globally estimated parameter ranges as the priors for a calibration with the local data or employing a hierarchical calibration approach (Tian et al., 2020, Fer et al., 2021), but the impact of these approaches should be separately researched and tested. Our study still successfully provided a global parameter set that increases the applicability of Yasso model and informs global SOC estimates.~~

How Yasso20 performs in comparison to Yasso07

When comparing the litter bag validation dataset performances of Yasso07 and Yasso20, there is an improvement with Yasso20 even though both models have been calibrated largely with the same litterbag data. This underlines that the added model detail and reconsidered calibration process have a positive impact on the model projections. What is more striking, though, is that Yasso20 does perform better across the board with the Hyytiälä SOC data than Yasso07 where the latter model's long term SOC component was calibrated with Finnish conditions. This result argues that while local calibration data is important, even for those specific locations there could be a benefit in including global data in the calibration. These results validate the third hypothesis concerning the impact of the presented improvements on model performance.

A more thorough analysis of the model projections revealed a more fundamental difference in the model dynamics than initially indicated by the comparison datasets. In Yasso07 the N pool decomposes much slower, which impacts the rest of the decomposition dynamics and causes less long-lived H pool carbon to be formed during the soil decomposition. As a consequence of differences in the calibration procedures and the resulting model versions, Yasso07 projects higher SOC values than Yasso20 with the same input values and these model versions would also react differently to changes in climate conditions and litter input.

The Yasso07 dynamics are most likely due to a combination of multiple reasons which highlights the complicated process of SOC model calibration. As Yasso07 was calibrated in segments, the woody decomposition parameters were calibrated after the AWENH pool parameters were determined from the global litter bag experiments and Finnish SOC measurements. When looking at the calibration results from individual datasets (Figure 2) there are parameter sets there which have similarly low decomposition rates for N pool as Yasso07. Depending on how the different measurement datasets were weighed, it might be that those datasets that favored slower N pool decomposition had more impact than with Yasso20 calibration. Finally, in Yasso20 the climate driver parameters are different between the AWE and N pools and while the temperature terms are close to each other, the precipitation terms do differ from each other while in Yasso07 they would be the same. This would affect the Yasso07 dynamics during calibration. The calibration is made even more vulnerable to all these factors because a vast majority of the litter bag data used here is from the first six years of decomposition where Yasso07 and Yasso20 are very close to each with regard to total carbon remaining (Figure 6). In such a situation it is very possible that less developed calibration protocols can lead to unrealistic system dynamics that still appear to produce good results within limited time windows.

Leaching

As established in section 2.2, in order to compare the measurements from different litter bag experiments, there needs to be a parameter that accounts for the litter bag types' impact on the mass loss rate (Tuomi et al., 2009). When testing with independent litterbag data, we see that even with this added assumption, the global calibration produces a better fit than the calibration based on individual litterbag campaigns (Table 5). This supports using data from multiple litterbag campaigns in model calibration. However, in the results it is evident that not only are the leaching parameters estimated to be essentially zero when calibrating only with individual decomposition bag data sets (Supplemental Table 5~~4~~), but also when simultaneously calibrating with all the data sets, only the ED dataset ends up having a meaningfully non-zero value. First of all, this indicates the current straight-forward formulation for leaching is insufficient as with the individual dataset calibrations the other parameter values are able to produce fits where there is no leaching despite knowledge that it is a factor. Second, even when calibrating multiple data sets simultaneously, the calibration appears to apply the leaching effect to only one of the datasets even when it should affect all of them.

~~Third, the~~A further complication is that the differences in RMSE results (Table 3) suggest that there are systematic differences between the datasets resulting from various sources such as the experimental setup or environmental differences. As a consequence, calibrating with these kinds of datasets will result in systematic differences in model performance as established in Oberpriller et al. (2021) as can be seen in how CIDET/LIDET calibrated Yasso performs with the ED dataset and vice versa. By being a corrective term, the leaching factor introduced here will also reflect all those other elements causing the systematic differences, for example different mycorrhizal environments, instead of just being about the physical properties of the litter bag. Due to all these factors,~~by being a corrective term, the leaching term will also reflect all other systematic differences between the datasets. As a consequence of all these factors,~~ the leaching impact needs to be further studied and the relevant equations need to first be formulated with experimental data specifically gathered for that purpose. There also needs to be additional work in trying to better quantify what those other systematic error elements are so that they can be better addressed.

Humus formation and the need for the layer Yasso

There is an important point concerning the parameterized humus (H) formation term p_H here. The long-term H formation can only take place in the soil itself as it requires the presence of mineral compounds (Schmidt et al., 2011), which is why only the global soil carbon dataset in this study could be used to constrain H parameters. However, they are only point measurements with no information of how the state changes over time. Therefore, we have to assume that the measurements represent the approximated steady state from an assumed litter fall. This not only causes larger parameter uncertainties, but also the estimated pH parameter value will represent the fraction of the total litter fall that ends up in the H pool while in reality with the surface vegetation litter there needs to be an additional mechanism that transfer the carbon compounds to soil while root litter is already in that environment. Consequently, if examining litter decomposition taking place only in the soil, such as with roots, it is likely that pH for that soil system would be larger than what is estimated here. This would fit with previous research suggesting that the root biomass specifically appears to be connected to the amount of long-term carbon in the soil as more of it would be able to form H compounds than the surface vegetation (Clemmensen et al., 2013; Jackson et al., 2017). However, currently the amount of data that would allow efficiently separating the above and below soil decomposition processes during the calibration process is limited. Additionally beyond this, there are presence of mineral compounds and other conditions that affect how efficiently H is formed that should be included when formalizing H formation (Rasmussen et al., 2018). Better addressing the formation of H is a crucial development step for the model, but the current approach provides an initial way to estimate the H pool size/quantity.

Temperature and precipitation impact

At first glance it appears that the current version of Yasso20 overestimates SOC decomposition (i.e. underestimates SOC amount) at higher precipitation and temperature values, as indicated by the negative trend in Fig 7~~3-4~~. In the current formulation of environmental drivers (eq. 5), only the lower precipitation values decrease the decomposition rate with the system becoming insensitive to increases in precipitation after a certain threshold. However, it is known that at higher moisture levels the SOC decomposition rates decrease (Keiluweit et al., 2017). A more informative driver of moisture conditions (e.g. monthly soil moisture) and a more realistic response function could help disentangle the reasons behind this trend in the residuals in the future. The current version of Yasso20 uses precipitation as the driver instead of soil moisture because the decomposition bags from the data sets used as constraints here are on the surface and thus were expected to be primarily controlled by precipitation. In the light of current findings, next steps in Yasso model development towards using soil moisture as model drivers are planned.

Closer examination of the error distribution over the climate drivers, though, suggests some more complexity. Even at the lower precipitation values while both CIDET and ED data errors cluster approximately equally around zero, the LIDET data points show a shift towards negative errors similarly to at higher precipitation values. Thus, it appears that the issue is at least partially due to the data set itself rather than the pure precipitation signal. Similar behaviour can be seen with mean temperature, although it isn't as pronounced. Thus, there is a seeming systematic error when simulating the LIDET data with the global calibration parameter sets. It is yet unclear if this is due to something with the measurements, something with the processes or if the climate driver data is not similarly representative of the conditions as with the other used data sets.

Litter size impact on decomposition

In the current Yasso20 implementation, the woody litter diameter does not change during the decomposition process while in reality the wood shrinks as it decomposes. This explains why when comparing the model results to the tree decomposition validation dataset (Fig 8~~3-5~~), the model overestimates the decomposition rate for decades old tree stems with a measured diameter of approximately 10 cm. In those cases, the model assumes that was the size of the trunks when the decomposition started and, consequently, the size impact is smaller than it should be. While the model still performs well with the validation database regardless of this, it is an important aspect to consider when applying Yasso20 model with woody decomposition.

5. Conclusions

Soil organic carbon (SOC) models should be constrained by data from multiple different ecosystems and reflecting the various dynamics affecting the SOC decomposition process. Using data from multiple datasets produced parameter sets which performed better in a global comparison than parameter sets calibrated with information from individual datasets, highlighting the necessity of using more data. However, the traditional AM calibration method had difficulties converging to a single parameter set when used with multiple datasets, most likely due to the numerous local likelihood maximas within the likelihood space, and our deliberate choice for avoiding detailed algorithm-specific configurations which reduces repeatability and re-applicability. Consequently, our results showed that more advanced methods such as DEzs should be used when calibrating SOC models. Furthermore, we identified numerous aspects where further detailed data is needed to better constrain the model processes in question, for example regarding the leaching parameter that allows comparison of different litter decomposition bag experiments or better connecting varying soil moisture conditions to changes in SOC.

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Author contributions

Dr. Toni Viskari came up with the study, planned the experiments and wrote majority of the manuscript. M.ScT. Janne Pusa did the simulations and the initial analysis of the results. Dr. Istem Fer participated in the experiment setup, analysis as well as wrote a part of the methodology. Drs. Anna Repo and Julius Vira provided insight to the data used and the mathematical aspects of the methods, respectively. Prof. Jari Liski is the PI of the project this research was a part of and has created the Yasso model used here.

Data availability

The Yasso model used here can be downloaded from https://github.com/YASSOmodel/Ryassofortran. The permanent version of the Yasso code, data used in this publication as well as the calibration algorithm has also been uploaded to Zenodo (10.5281/zenodo.5059909). The manual on the calibration process is within the calibration folder.

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Parameter symbol	Parameter description	Prior distributions	Starting values
α_A	Base decomposition rate for pool A (1/year)	U(0,2)	1.86, 0.23, 1.37
α_W	Base decomposition rate for pool W (1/year)	U(0,10)	3.52, 6.0, 9.74
α_E	Base decomposition rate for pool E (1/year)	U(0,2)	0.36, 1.63, 0.82
α_N	Base decomposition rate for pool N (1/year)	U(0,0.1)	0.01, 0.06, 0.03
α_H	Base decomposition rate for pool H (1/year)	U(0.001,0.01)	0.0024, 0.0094, 0.0045
p_{AW}	Transference fraction from pool A to pool W	U(0,1)	Set value of 1-p_H
p_{AE}	Transference fraction from pool A to pool E	U(0,1)	Set value of 0
p_{AN}	Transference fraction from pool A to pool N	U(0,1)	Set value of 0
p_{WA}	Transference fraction from pool W to pool A	U(0,1)	0.31, 0.37, 0.68
p_{WE}	Transference fraction from pool W to pool E	U(0,1)	Set value of0
p_{WN}	Transference fraction from pool W to pool N	U(0,1)	0.42, 0.45, 0.20
p_{EA}	Transference fraction from pool E to pool A	U(0,1)	Set value of 1-p_{EW}-p_H
p_{EW}	Transference fraction from pool E to pool W	U(0,1)	0.47, 0.91, 0.04
p_{EN}	Transference fraction from pool E to pool N	U(0,1)	Set value 0.
p_{NA}	Transference fraction from pool N to pool A	U(0,1)	Set value of 1-p_H
p_{NW}	Transference fraction from pool N to pool W	U(0,1)	Set value of 0
p_{NE}	Transference fraction from pool N to pool E	U(0,1)	Set value of 0
p_H	Transference fraction from AWEN pools to pool H	U(0.001,0.01)	0.0071, 0.0064, 0.0026
β_1	The first order temperature parameter for AWE pools (1/C)	U(0,0.2)	0.03, 0.04, 0.17
β_2	The second order temperature parameter for AWE pools (1/C^2)	U(-0.05,0)	-0.013, -0.007, -0.003
β_{N1}	The first order temperature parameter for N pool (1/C)	U(0,0.2)	0.12, 0.01, 0.02
β_{N2}	The second order temperature parameter for N pool (1/C^2)	U(-0.05,0)	-0.24, -0.04, -0.03
β_{H1}	The first order temperature parameter for H pool (1/C)	U(0,0.2)	0.002, 0.11, 0.20
β_{H2}	The second order temperature parameter for H pool (1/C^2)	U(-0.05,0)	-0.0001, -0.0014, -0.39
Γ	The precipitation impact parameter for AWE pools (year/mm)	U(-2,0)	-0.93, -1.96, -1.34
γ_N	The precipitation impact parameter for N pool (year/mm)	U(-2,0)	-1.66, -0.32, -0.63
γ_H	The precipitation impact parameter for H pool (year/mm)	U(-10,-5)	-9.65, -6.15, -5.47
ϕ_1	The first order impact parameter for size (1/cm)	U(-3,0)	-0.81, -1.41, -1.19

ϕ_2	The second order impact parameter for size (1/cm^2)	U(3,0)	0.82, 0.25, 2.25
r	The exponent parameter for size	U(0,1)	0.83, 0.17, 0.49
w_{ED}	The leaching parameter for ED dataset	U(-1,0)	-0.08, -0.02, -0.05
w_{CIDET}	The leaching parameter for CIDET dataset	U(-1,0)	-0.03, -0.1, -0.08
w_{LIDET}	The leaching parameter for LIDET dataset	U(-1,0)	-0.08, -0.04, -0.02

Table 1: The parameters, prior distributions and initial values used in this calibration study. The initial values for the different chains were randomly drawn from the prior distribution (U: uniform). If the starting value is listed as a set value, then parameter was not varied in the calibration and the given value was used for all chains.

Data	N	No. of Species	Time range (a)	T range (°C)	P range (mm)	Elevation range (m)	Uncertainty used in calibration	Note	Reference
Non-woody litter decomposition								Mesh size (cm)	
CIDET	1259	10	0-6	-9.8–9.3	261–1782	48–1530	100g	0.25 x 0.5	Trofymow 1995
LIDET fine roots	2608	4	0-10	-7.4–26.3	150–3914	0–3650	200g	0.055 x 0.055	Gholz et al. 2000
LIDET litter	5900	29	0-10	-7.4–26.3	150–3914	0–3650	200g	0.055 x 0.056	Gholz et al. 2001
EURODECO	2184	5	0-5.5	0.2–7	469–1067	46–350	A:40g, W:10g, E: 20g, N:40g	1 x 1	Berg et al. 1991a, b
Hobbie	192	4	0-5	6.7	3676	270	100g	0.3 x 0.2	Hobbie 2005
Woody litter decomposition								Diameter (cm)	
Finland	1281	3	0-60	3.1	570	na	250g	4.5–40.9	Mäkinen et al. 2006
SOC accumulation								Soil depth (cm)	
Finland	26		5300	3	500	0	NA	0–30	Liski et al. 2005
SOC stock									
Global	4113			-26.9–28.0	0–5663	0–3900	7.5 kg	0–100	Zinke et al. 1986
Finland	30			3.2	681	115–180	NA	0–100	Liski & Westman 1995
Total	17563								

Table 2: The measurement data sets used in this research

	~~DEzs MAP~~	~~DEzs G-R~~	~~DREAMzs MAP~~	~~DREAMzs G-R~~	~~AM MAP~~	~~AM G-R~~
~~αA~~	~~0.51~~	~~1.01~~	~~0.46~~	~~1.06~~	~~**0.53**~~	~~**1.15**~~
~~αW~~	~~5.19~~	~~1.01~~	~~4.7~~	~~1.06~~	~~**5.37**~~	~~**1.17**~~
~~αE~~	~~0.13~~	~~1.01~~	~~0.11~~	~~1.04~~	~~**0.13**~~	~~**1.23**~~
~~αN~~	~~0.10~~	~~1.01~~	~~0.1~~	~~1.05~~	~~**0.1**~~	~~**1.31**~~
~~αH~~	~~0.001~~	~~1.02~~	~~0.002~~	~~1.02~~	~~0.002~~	~~1.07~~
~~pWA~~	~~0.5~~	~~1.00~~	~~0.5~~	~~1.03~~	~~0.50~~	~~1.04~~
~~pWN~~	~~0.16~~	~~1.01~~	~~0.17~~	~~1.08~~	~~0.16~~	~~1.06~~
~~pEW~~	~~0.99~~	~~1.02~~	~~0.97~~	~~1.09~~	~~0.98~~	~~1.09~~
~~pH~~	~~0.004~~	~~1.01~~	~~0.004~~	~~1.04~~	~~0.005~~	~~1.00~~
~~wED~~	~~-0.19~~	~~1.01~~	~~-0.18~~	~~1.03~~	~~-0.19~~	~~1.03~~
~~wCIDET~~	~~-0.03~~	~~1.01~~	~~-0.02~~	~~1.04~~	~~-0.02~~	~~1.04~~
~~wLIDET~~	~~0.~~	~~1.01~~	~~0.~~	~~1.01~~	~~0.~~	~~1.04~~
~~β1~~	~~0.16~~	~~1.00~~	~~0.17~~	~~1.08~~	~~**0.16**~~	~~**1.30**~~
~~β2~~	~~-0.002~~	~~1.00~~	~~-0.002~~	~~1.07~~	~~**-0.002**~~	~~**1.48**~~
~~β1N~~	~~0.17~~	~~1.00~~	~~**0.18**~~	~~**1.12**~~	~~**0.19**~~	~~**1.28**~~
~~β2N~~	~~-0.005~~	~~1.00~~	~~**-0.005**~~	~~**1.13**~~	~~**-0.006**~~	~~**1.38**~~
~~β1H~~	~~0.07~~	~~1.02~~	~~**0.07**~~	~~**1.15**~~	~~**0.07**~~	~~**1.55**~~
~~β2H~~	~~0.~~	~~1.02~~	~~**0.**~~	~~**1.18**~~	~~**0.**~~	~~**1.28**~~
~~ɣ~~	~~-1.44~~	~~1.01~~	~~-1.66~~	~~1.09~~	~~**-1.58**~~	~~**1.30**~~
~~ɣN~~	~~-2.0~~	~~1.04~~	~~-2.0~~	~~1.07~~	~~**-1.99**~~	~~**1.19**~~
~~ɣH~~	~~-6.9~~	~~1.01~~	~~-5.78~~	~~1.09~~	~~**-8.56**~~	~~**1.30**~~
~~ϕ1~~	~~-2.55~~	~~1.01~~	~~-2.32~~	~~1.03~~	~~**-2.64**~~	~~**2.88**~~
~~ϕ2~~	~~1.24~~	~~1.01~~	~~1.18~~	~~1.05~~	~~**1.32**~~	~~**2.69**~~
~~R~~	~~0.25~~	~~1.01~~	~~0.25~~	~~1.05~~	~~**0.25**~~	~~**2.08**~~

~~Table 3 The estimated parameter value MAPs and Gelman-Rubin coefficients for DEzs, DREAMzs and AM for global calibration against all data streams. Parameter that did not pass the G-R test are bolded.~~

~~Parameter~~	~~Global~~	~~CIDET~~	~~LIDET~~	~~ED~~
~~αA~~	~~0.51~~	~~1.33~~	~~0.60~~	~~0.58~~
~~αW~~	~~5.19~~	~~9.95~~	~~9.40~~	~~5.74~~
~~αE~~	~~0.13~~	~~0.14~~	~~0.00~~	~~0.17~~
~~αN~~	~~0.10~~	~~0.02~~	~~0.08~~	~~0.10~~
~~αH~~	~~0.0015~~	~~–~~	~~–~~	~~–~~
~~pWA~~	~~0.50~~	~~0.59~~	~~0.59~~	~~0.41~~
~~pWN~~	~~0.16~~	~~0.08~~	~~0.06~~	~~0.16~~
~~pEW~~	~~0.99~~	~~0.26~~	~~0.42~~	~~0.97~~
~~pH~~	~~0.0042~~	~~–~~	~~–~~	~~–~~
~~wED~~	~~-0.19~~	~~–~~	~~–~~	~~0.~~
~~wCIDET~~	~~-0.03~~	~~0.~~	~~–~~	~~–~~
~~wLIDET~~	~~0.~~	~~–~~	~~0.~~	~~–~~
~~β1~~	~~0.16~~	~~0.19~~	~~0.13~~	~~0.19~~
~~β2~~	~~-0.002~~	~~-0.003~~	~~-0.001~~	~~0.~~
~~β1N~~	~~0.17~~	~~0.19~~	~~0.19~~	~~0.20~~
~~β2N~~	~~-0.005~~	~~0.~~	~~-0.003~~	~~0.~~
~~β1H~~	~~0.07~~	~~–~~	~~–~~	~~–~~
~~β2H~~	~~0.~~	~~–~~	~~–~~	~~–~~
~~γ~~	~~-1.44~~	~~-0.46~~	~~-1.74~~	~~-0.88~~
~~γN~~	~~-2.0~~	~~-1.2~~	~~-0.06~~	~~-1.57~~
~~γH~~	~~-6.9~~	~~–~~	~~–~~	~~–~~
~~ϕ1~~	~~-2.55~~	~~–~~	~~–~~	~~–~~
~~ϕ2~~	~~1.24~~	~~–~~	~~–~~	~~–~~
~~r~~	~~0.25~~	~~–~~	~~–~~	~~–~~

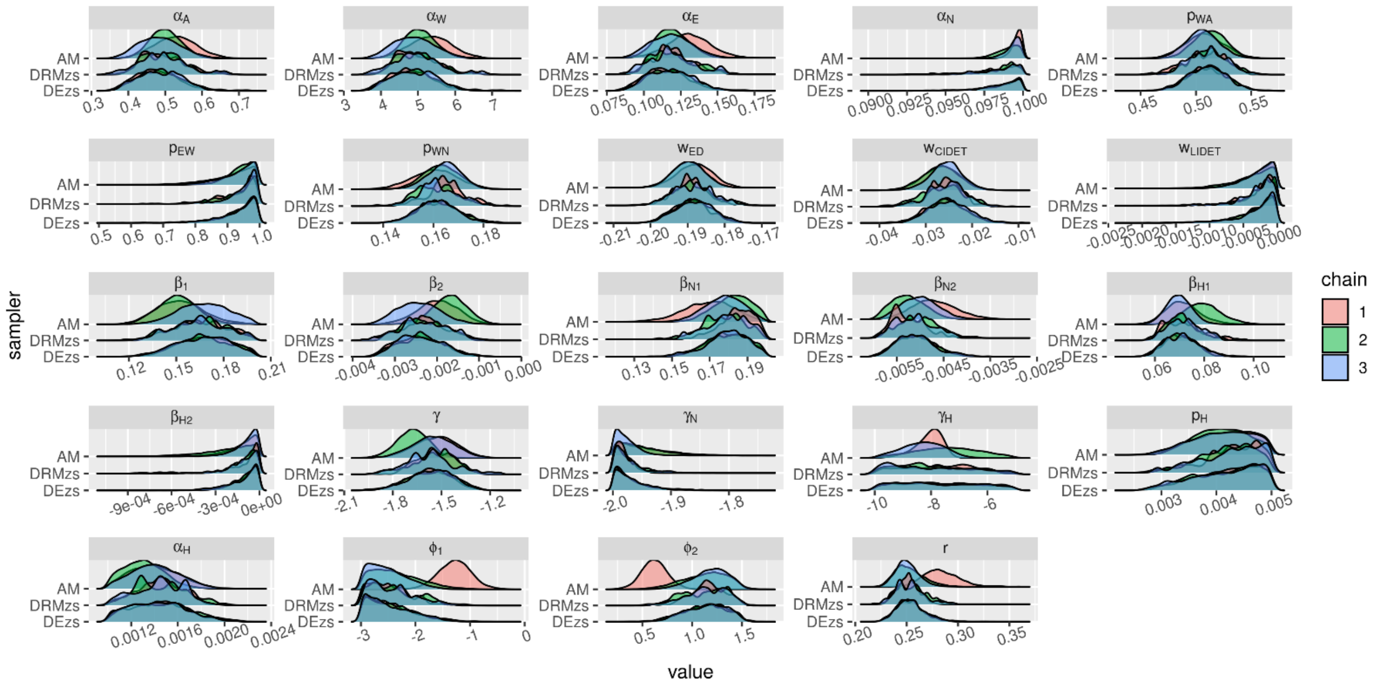
~~Table 4 Estimated parameter MAP values with DEzs approach using all the datasets opposed to the individual litter decomposition experiments in the calibration~~

Validation dataset	CIDET calibration	LIDET calibration	ED calibration	Global calibration
CIDET	**109.0**	128.8	226.4	115.5
LIDET	224.3	**168.8**	345.4	199.9
ED	49.5	55.0	**35.5**	40.3
Hob3	133.8	126.6	367.0	**110.0**

Table 3~~5~~. The RMSE values for the different validation datasets when the model is ran with the MAP values from the calibrations done with the different datasets. As with the measurements, the RMSE unit here is grams. Lowest RMSE for a particular dataset is bolded.

Site ID (Dominant tree species; Number of plots)	Averaged SOC (Standard deviation)	Yasso20 ~~P~~projected steady state SOC	Yasso07 projected steady state SOC
CT_SP (Pine; 5)	5.78 (0.97)	5.82	8.32
VT_SP (Pine; 7)	5.73 (0.71)	7.39	10.61
VT_NS (Spruce; 2)	6.86 (0.67)	8.78	13.06
MT_SP (Pine; 4)	6.89 (1.93)	8.80	12.78
MT_NS (Spruce; 7)	8.61 (0.84)	9.26	13.87
OMT_NS (Spruce; 5)	9.6 (2.2)	10.26	15.47

Table 4~~6~~: Both averaged measured SOC and projected SOC values with both Yasso07 and Yasso20 for forest plots in Hyytiälä, Finland classified by measurement site. All the units are in kgC m^{-2}.



965 Figure 1: The global calibration results with the different calibration methods.

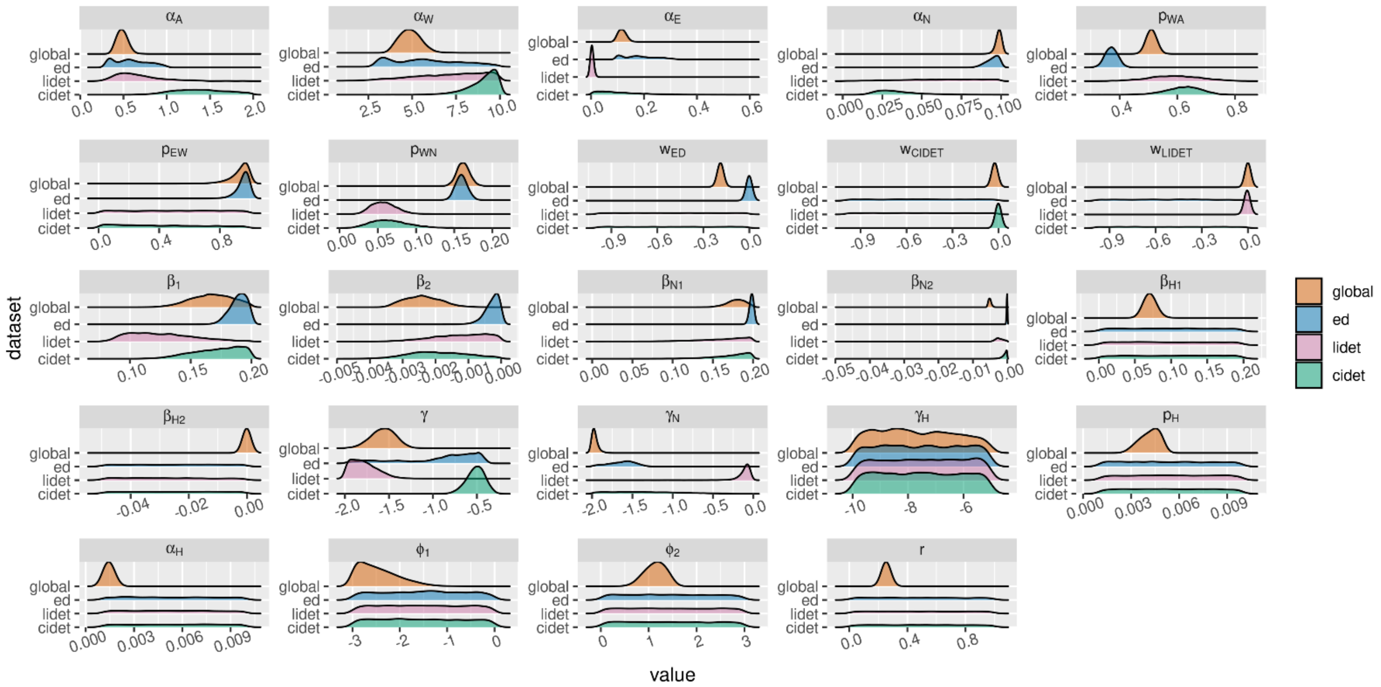


Figure 2: The estimated parameter distributions using DEzs with different calibration data sets.

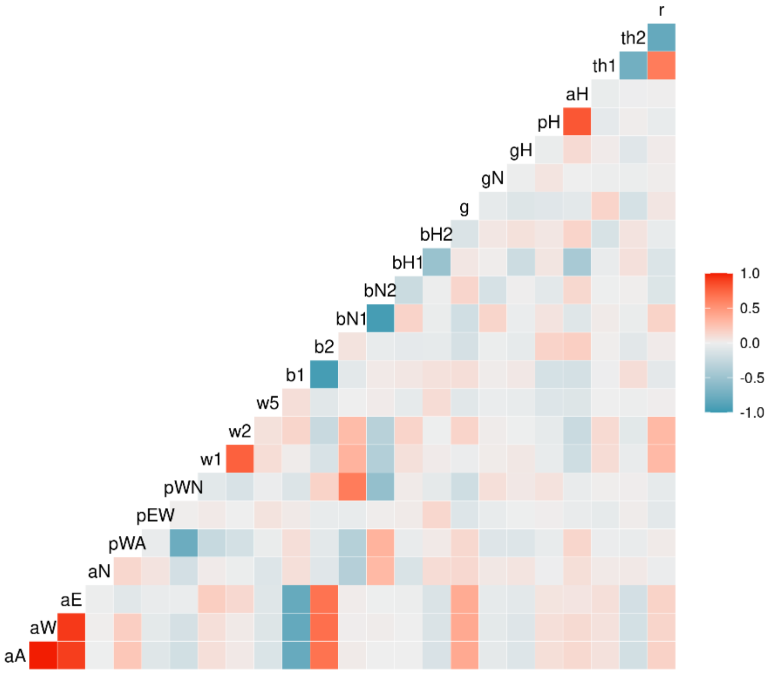
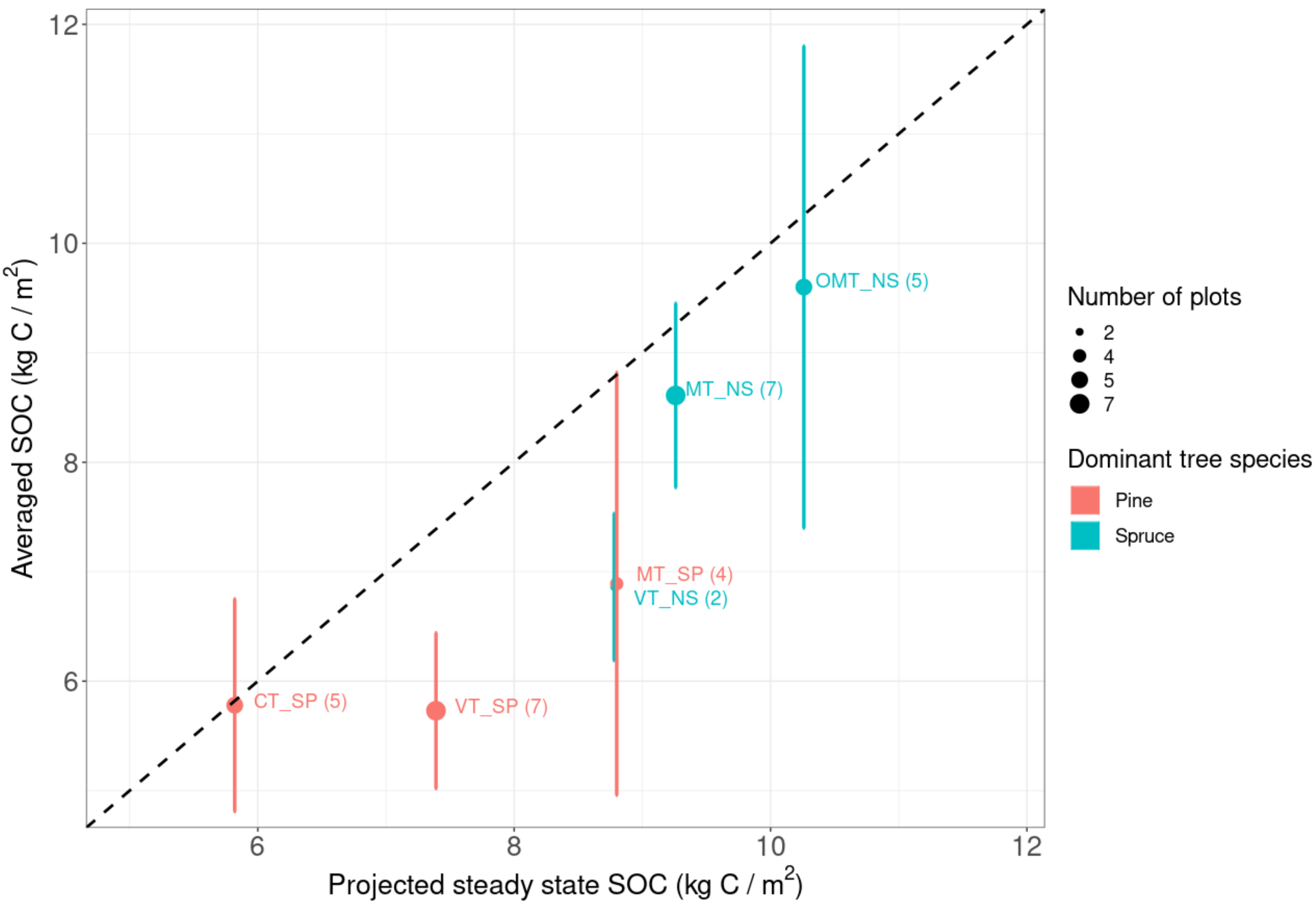


Figure 3: Parameter correlations for the global calibration with the DEzs algorithm.



975

Figure 4~~3~~: The projected steady state SOC compared to the averaged measured SOC values in plots from multiple measurement sites.

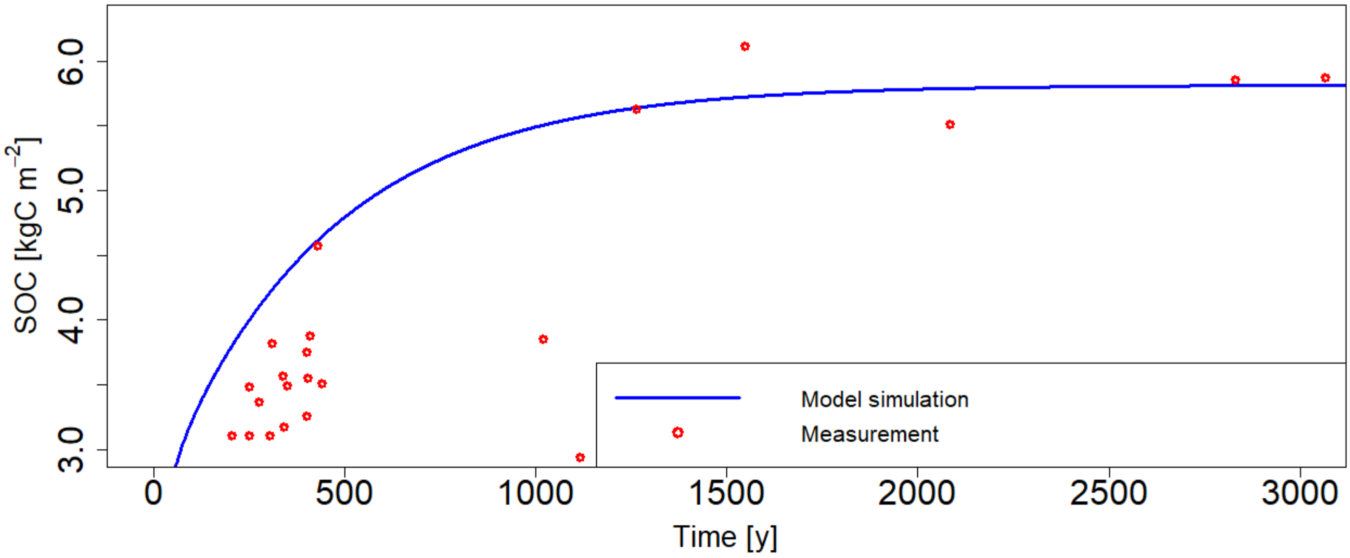


Figure 54: Measurement (Red dots) and model (Blue line) based projections of SOC accumulation on the Finnish coast after the end of ice age.

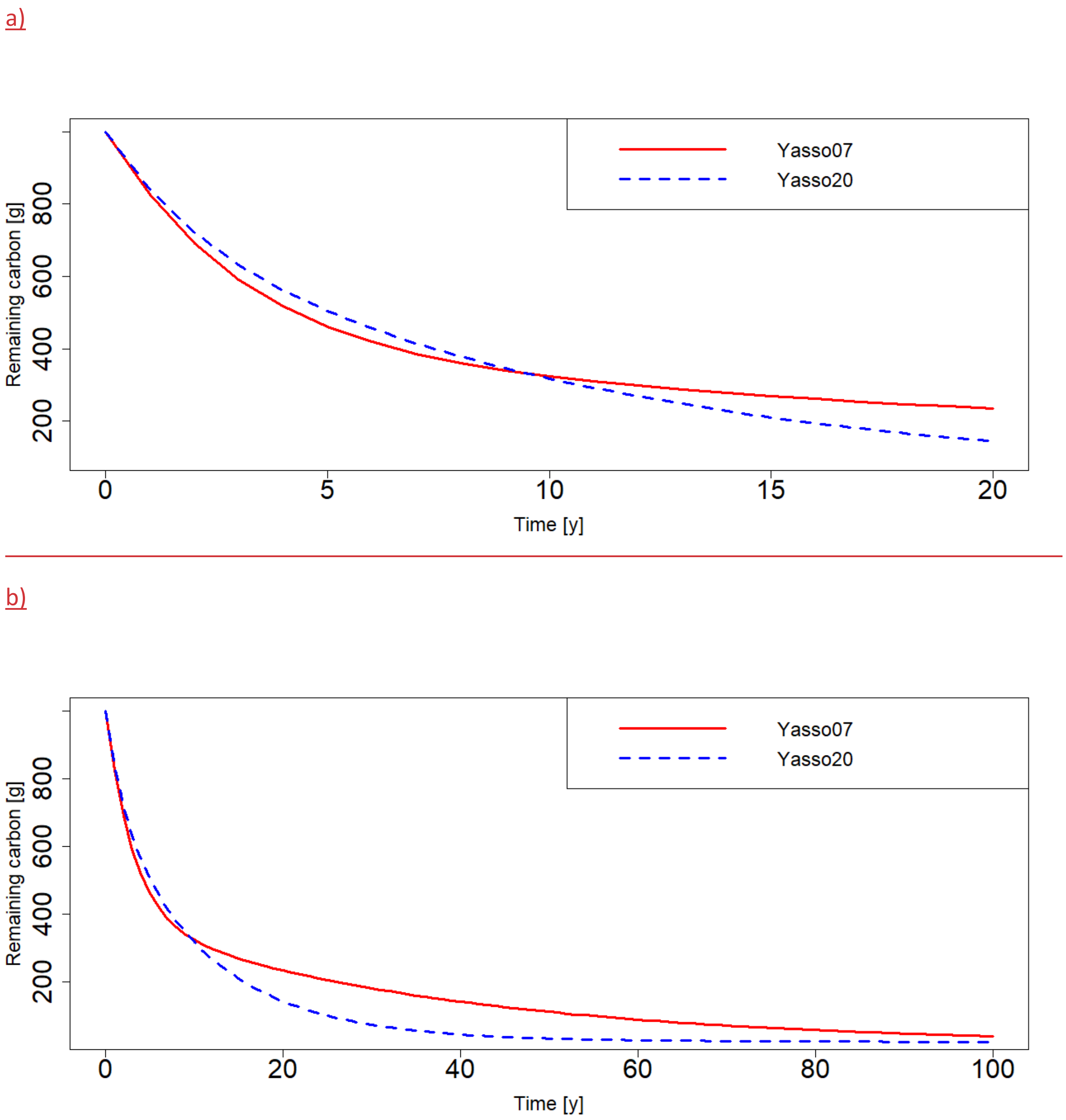


Figure 6: The remaining decomposing carbon for a hypothetical straw litter in Hyytiälä, Finland climate condition when simulated with Yasso07 (solid red) and Yasso20 (dashed blue) with a) 20 year and b) 100 year time window.

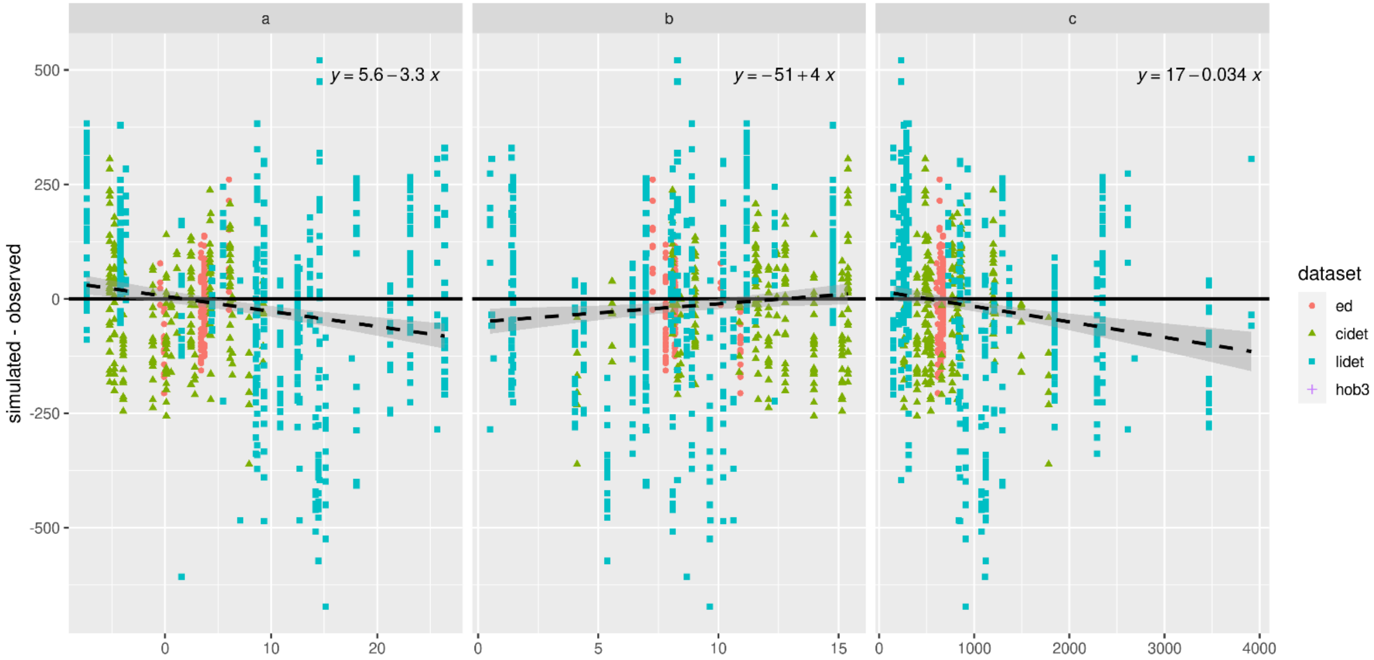


Figure 7~~65~~: Residual analysis between simulated and observed carbon remnant on a) mean temperature (C), b) temperature variation (C) and c) total precipitation (mm y^{-1}) at the validation site.

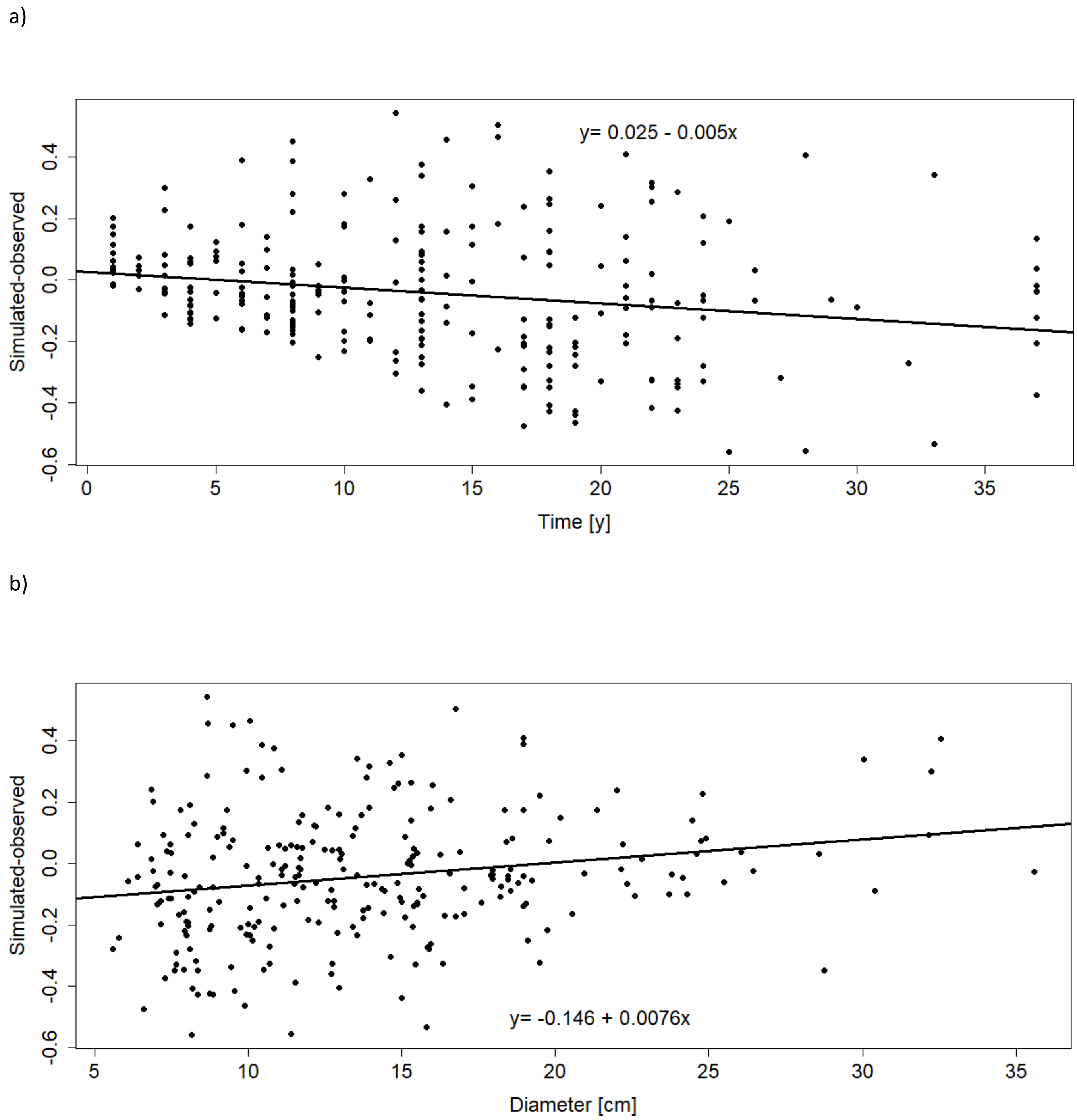
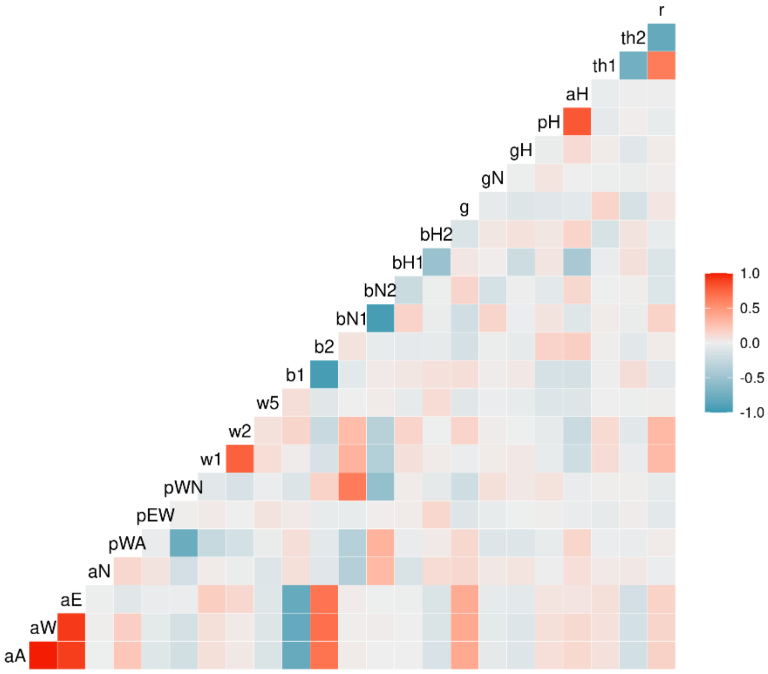


Figure 8~~76~~: Residual analysis between simulated and observed carbon remnants of wood decomposition from Mäkinen et al. (2006) on a) decomposition time and b) diameter.



~~Figure 7: Parameter correlations for the global calibration with the DEzs algorithm.~~