A robust DayCent model calibration to assess the potential impact of integrated soil fertility management on maize yields, soil carbon stocks and greenhouse gas emissions in Kenya.

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Abstract. Sustainable intensification schemes that increase erop production and soil fertility, such as integrated soil fertility management (ISFM) , are a proposed strategy to close yield gaps, increase soil fertility, and achieve food security in sub-Saharan Africawhile maintaining soil fertility. However, field trials are insufficient to estimate the potential impact of such technologies at the regional or national scale. Upscaling via biogeochemical models , , Biogeochemical models such as Day-

- 5 Cent, from the field-scale to a larger region can be a suitable and powerful way to assess the potential of such agricultural management practices at scalecan assess their potential at larger scales, but they need to be calibrated to new environments and their reliability needs to be assuredrigorously tested for accuracy. Here, we present a robust Bayesian calibration of Day-Cent to simulate maize productivity and soil organic carbon stock changes under ISFM, using data from four long-term field experiments in Kenya in a leave-one-site-out cross-evaluation approach. The experimental treatments consisted of the addition
- 10 of low- to high-quality organic resourcesto the soil, with and without mineral N fertilizer. We assesses assessed the potential of DayCent to accurately represent the key aspects of sustainable intensification, including 1) yield, 2) the changes in soil carbon, and 3) global warming potential. The model was calibrated and cross-evaluated with the probabilistic Bayesian calibration technique the greenhouse gas (GHG) balance of CO₂ and N₂O combined.

The standard parameters of DayCent led to poor calibration with cross-evaluation improved DayCent simulations of maize 15 yield(, evaluated across all sites, (from a Nash–Sutcliffe modeling efficiency ; EF0.33) and changes in SOC(EF -1.3)for

different ISFM treatments. After calibration of the model, both (EF) of 0.36 to 0.50) but slightly worsened those of soil organic carbon (SOC) (from EF of 0.36 to 0.34). By site, the simulation of maize yield (EF 0.51) and the change in SOC (EF 0.54)improved significantly compared to the model with the standard parameter values. A leave-one-site-out improved

(to site-specific EF between 0.16 and 0.39) and that of SOC slightly worsened (to site-specific EF between -1.8 and 0.39).

20 The model performance and the match between the cross-evaluation posterior credibility intervals for different sites indicated

the robustness of the approach-model parameterization and the reliability of the Daycent model for spatial upscaling (i. e., the significant improvement, described before, was achieved by calibrating with data from 3 sites and evaluating with the remaining of simulations. While daily N₂O emissions were poorly reproduced by DayCent (all EF values were negative), cumulative seasonal N₂O emissions were simulated more accurately (EF ranging between 0.03 and 0.62 by site). The SOC

- 25 decomposition parameters were altered most severely by the calibration. They were an order of magnitude higher compared to the default parameter set. This confirms that the decomposition of SOC in tropical maize cropping systems is much faster than in temperate systems and that the DayCent temperature function is not suitable to capture this with a single parameter set. Finally, the global warming potential simulated by DayCent simulated yield-scaled GHG balance was highest in control -N treatments (treatments without N addition (between 0.5 -2.5 and 1.5 kg CO₂ equivalent per kg grain yield , depending on the
- 30 site) and could be reduced by 14 to 72 across sites) and was lower by about 10 to 60% by combined application of mineral N and manure at a medium rate. In three of the four sites, the global warming potential was largely $(2.75%)$ dominated by SOC losses. In summary moderate rate of $1.2tC$ ha⁻¹ yr⁻¹. In conclusion, our results indicate that DayCent is suitable for estimating well-suited to estimate the impact of ISFMfrom the site to the regional level, that trade-offs between yields and global warming potential are , that the trade-off between maize yield and GHG balance is stronger in low-fertility sites, and that the reduction
- 35 control of SOC losses is a priority for the sustainable intensification of maize production in Kenya.

1 Introduction

Similar to many countries of In Kenya, as in many other Sub-Saharan Africa (SSA) countries, maize yields have remained low, the low maize yields in Kenya, on average 1.7 t ha⁻¹ compared to the global average of 5.6 t ha⁻¹ over the last decade (2011-2021) [\(FAO, 2023\)](#page-52-0), are in part responsible for (2011-2021; [FAO, 2023\)](#page-52-0). This contributes to the low self-sufficiency

- 40 of food production. Consequently, with around 20% of the Kenyan population lives with facing severe food insecurity [\(World-Bank, 2021b\)](#page-57-0). If yields are not improved, increased demand due to population growth will further deteriorate food self-sufficiency and in general food security in general in the coming decades [\(Zhai et al., 2021\)](#page-57-1): especially considering expected yield declines resulting from more frequent extreme weather events could further exacerbate this situation [\(Lobell](#page-54-0) [et al., 2011\)](#page-54-0). One of the key limitations to sustainable maize production in SSA is the lack insufficient use of mineral fer-
- 45 tilizer and organic inputs [\(Vanlauwe et al., 2010\)](#page-56-0). Integrated soil fertility management (ISFM) is a sustainable intensification practice that can alleviate these limitations by combining the use of mineral fertilizers with organic inputs [\(Vanlauwe et al.,](#page-56-0) [2010\)](#page-56-0). Different studies Several studies have reported that ISFM has the potential to more than double maize yields in Kenya, especially in currently unfertile on infertile soils, due to the effects its positive impact on soil fertility, including soil organic matter (SOM) content [\(Chivenge et al., 2009,](#page-51-0) [2011\)](#page-51-1). However, in addition to the amount and quality of fertilizer and organic
- 50 inputs, Furthermore, increasing SOM can help mitigate adverse effects of climate change, offering considerable potential in carbon-depleted soils across SSA [\(Corbeels et al., 2019\)](#page-51-2). However, the effectiveness of ISFM in increasing yields strongly depends on local site conditions, such as soil and climate [\(Chivenge et al., 2011\)](#page-51-1). Furthermore, increasing SOM also contributes

to minimizing the negative effects of climate change, and there may be considerable potential in carbon-depleted soils in SSA [\(Corbeels et al., 2019\)](#page-51-2).

- 55 Hence, to _{Lo} close yield gaps in a resource-efficient way and to assess the climate change mitigation potential of ISFM, we need to understand the effects of long-term implementation of ISFM at larger scaleslong-term effects of ISFM practices at a larger scale. Ideally, this would be facilitated by implementing a large number of long-term experiments (LTE) across a representative range of soil and climatic conditions. However, due to the high demands in terms of costthe significant costs, labor, and time associated with maintaining LTE, required to maintain long-term experiments limit the number of LTE that
- 60 evaluate variation in the sites for evaluating the variable effects of ISFM practices due to under site-specific conditionsis very limited. In addition, using relying on statistical predictive techniques to upscale results obtained with a low from a limited number of sites could may lead to low predictive power and large predictive errors, because it is unlikely that the effects of variation in soils and climate on yield and the development of soil organic matter (SOM) SOM would be fully captured by in the statistical models.
- 65 Biogeochemical process-based ecosystem models, such as DayCent [\(Parton et al., 1998;](#page-55-0) [Del Grosso et al., 2001\)](#page-52-1), are able to simulate the influence of simulate the effects of important driving variables of on crop yield and SOM formation using semimechanistic functions developed through decades of agronomic and soil research. Because they (partly) embed our current [u](#page-56-1)nderstanding of the complex ecosystem processes, they are more robust for upsealing of scaling up the yield potential [\(Saito](#page-56-1) [et al., 2021\)](#page-56-1) and the SOM building capacity [\(Lee et al., 2020\)](#page-54-1), compared to statistical predictive techniques. However, to
- 70 avoid bias in model output, it is best practice that models are calibrated and validated to local conditions [\(Necpálová et al.,](#page-55-1) [2015\)](#page-55-1)whenever they are applied outside the range of usual conditions, for example, in a new climate zone , especially when applied in novel contexts such as different climate zones with different soils.

Although DayCent has been used to estimate the development of SOM stock-SOM stock changes in Kenya on a national scale [\(Kamoni et al., 2007\)](#page-53-0)and recently the efficiency , and recently to assess the impact of conservation agriculture on SOM in

- 75 Ethiopia [\(Lemma et al., 2021\)](#page-54-2), DayCent's its modules of SOM and maize crop growth have never been rigorously calibrated and validated for tropical agroecosystems in SSA. A recent test evaluation of DayCent in Kenyan maize growing systems showed that SOM turnover is underpredicted by DayCent the model [\(Nyawira et al., 2021\)](#page-55-2). Because SOM in biogeochemical models is coupled to nitrogen (N) mineralization in biogeochemical models, there is the potential that this translates into biased crop responses to N addition and biased crop growth rates productivity predictions in any upscaling exercise. A potential solution
- 80 to this issue is the joint simultaneous calibration of soil and crop parameters in DayCent , using long-term using data from local trialslong-term experiments. Ideally, it this calibration would include the uncertainty in the model parameters and model outputs [\(Clifford et al., 2014\)](#page-51-3), so a propagation of errors is possible in upscaling exercises [\(Stella et al., 2019\)](#page-56-2). This is especially relevant because given a recent study showed showing considerable uncertainty in DayCent's SOM turnover rates, even when calibrated using a range of long-term experiments for calibration (Gurung et al., 2020).
- 85 In order to use DayCent to assess the potential of ISFM to contribute to closing the yield gap reduce yield gaps while minimizing environmental impact in Kenya and other SSA countries, the aim of this study was to use this study used a Bayesian calibration to derive robust DayCent parameters of SOM cycling and maize growth in Kenya. With robust, we

mean that the model evaluation statistics are representative of applying the model to new sites with the same climate and soils. We used the experimental data of four long-term ISFM trials experiments conducted in Kenya for almost two decades

- 90 [\(Laub et al., 2022a,](#page-53-1) [2023b\)](#page-54-3) over nearly two decades [\(Laub et al., 2023a,](#page-54-4) [b\)](#page-54-3). Of these, two sites were in humid western Kenya and two in subhumid to semi-arid central Kenya. Their treatments were different additions of organic resources (1.2 and 4 t C ha-1 yr-1 including farmyard manure, high-quality *Tithonia diversifolia* and *Calliandra calothyrsus* residues as well as low-quality low quality stover of *Zea mays* and sawdust), combined with (+N) or without (-N) 120 kg mineral N fertilizer ha-1 season⁻¹. They thus contain a range of experimental conditions and inputs. The goal
- 95 The first objective of our study was to evaluate to what extent DayCent can replicate reproduce the differences in yields and SOM development in response to the addition of different qualities and rates of organic resources combined with different rates of N fertilizer and between sites. Furthermore, because ISFM can simultaneously be a source of N_2O to the atmosphere [\(Leitner et al., 2020\)](#page-54-5) and mitigate CO_2 emissions from the soil [\(Laub et al., 2022a\)](#page-53-1), the for a number of contrasting sites. The second objective was to evaluate the total global warming potential of different greenhouse gas (GHG) balance of different
- 100 addition rates of organic material in ISFM to find the optimal balance between limiting greenhouse gas GHG emissions from the soil and optimizing the crop yield (that is, sustainable intensification). ISFM can be a source of N₂O to the atmosphere [\(Leitner et al., 2020\)](#page-54-5) but at the same time mitigate CO₂ emissions due to the mineralization of SOC [\(Laub et al., 2023a\)](#page-54-4).

Thus, the specific The specific steps to reach the objectives of this study were (i) to test the capability of an uncalibrated version of DayCent to simulate yield and SOC development of the different ISFM practices, (ii) to calibrate DayCent to represent

105 ISFM under Kenyan conditions using experimental data from the 4 LTEfour long-term experiments, displaying the confidence in model parameters by Bayesian calibration, and (iii) to use the calibrated model to gain an understanding of possible trade-offs between yield and SOM increases under ISFM, and to understand the global warming potential understanding of the GHG balance of the different ISFM treatments.

2 Material and Methods

110 2.1 The experimental sites

The present study used data pooled from four experimental sites. The experiments tested different organic resource treatments from four long-term field experiments in Kenya, in which the effect of the addition of different organic resources at different rates was tested, either alone or in combination with the application of mineral N fertilizer, in the context of ISFM. The experimental setup was identical between the sites . The sites sites are located in agriculturally important areas in western

- 115 and central Kenya. central and western Kenya (Fig. [A1\)](#page-41-0). The Embu and Machanga sites are both located in Embu County, in the central part of Kenya. The Aludeka site is located situated in Busia County in western Kenya, while Sidada is located in the adjacent Siaya County, just south of Busia (Table [A1\)](#page-38-0). The experiments in Embu and Machanga were initiated began in early 2002and the experiments , while those in Aludeka and Sidada were initiated began in early 2005. Therefore, 19 years of data were available in central Kenya and 16 years in western Kenya (2 sites x 16 years + 2 sites x 19 years = 70 site years
- 120 $\frac{\text{site}^* \text{years}}{\text{size}^* \text{years}} = 140 \text{ site} \cdot \text{seasons}$ and $\frac{\text{size}^* \text{years}}{\text{size}^* \text{years}} = 140 \text{ site} \cdot \text{seasons}$. The sites cover a range of altitudes, temperatures, and precipitations. Embu, with a

mean annual temperature (MAT) of 20 °C and an annual precipitation of 1200 mm annual precipitation mm, is the coolest of all sitessite, while Machanga has a MAT of 24°C and receives the lowest amounts of the lowest annual precipitation (800 mm). Sidada (23°C, 1700 mm) and Aludeka (24°C, 1700 mm) have a high MAT and receive significantly more precipitation than the sites in central Kenya. There are two rainy seasons at each site, which corresponds corresponding to two maize growing

125 seasons per year. The long rainy season *runs occurs* from March to August /September, or September, while the short rainy season runs occurs from October until January *lor* February. In terms of soil texture, Machanga and Aludeka have low clay content (13% clay at both sites), while Sidada and Embu are rich in clay (56 and 60%, respectively).

All experiments were set up as a split plot design with three replicates, with different qualities and quantities of organic resources as main plots and the presence or absence of N fertilizer as subplots. Maize was grown continuously in all experiments,

- 130 with two crops per year, one in the long rainy season and one in the short rainy season. The **design was similar in** experimental design was identical at all four sites and has been described in detail for the Embu site [\(Chivenge et al., 2009;](#page-51-0) Gentile et al., 2011) in earlier publications [\(Chivenge et al., 2009;](#page-51-0) [Gentile et al., 2011;](#page-52-3) [Laub et al., 2023a,](#page-54-4) [b\)](#page-54-3). Organic resource treatments consisted of high quality *Tithonia diversifolia* (TD) green manure and *Calliandra calothyrsus* (CC) prunings, low quality stover of *Zea mays* (MS) and sawdust from *Grevillea robusta* trees (SD), locally available farmyard manure (FYM) and a control treatment
- 135 (CT) without any organic resource additions. Organic resources differed in quality by the contents of N, lignin and polyphe-nols (Table [A2\)](#page-39-0). Each organic resource was applied once a year at two rates, 1.2 and 4 t C ha⁻¹ yr⁻¹, while only one amount of applied mineral fertilizer, mineral N fertilizer was applied at a fixed rate of 120 kg N ha⁻¹ (CaNH₄NO₃) in each of the two growing seasonswas tested. Of that Of this, 40 kg N ha⁻¹ were applied with at planting, and the remaining 80 kg N ha⁻¹ about six weeks after plantinglater. Organic resources were applied only once a year, prior to planting for in the long rainy season,
- 140 i.e., in January or February. They were incorporated to a depth of 15 cm with hand hoes. Furthermore, a blanket application of 60 kg P ha⁻¹ as triple superphosphate and of 60 kg K ha⁻¹ as muriate potash at planting was provided to all plots once each season. The plots were kept weed free by hand weeding, between two and two to three times per season, and selective application of pesticides was used when necessary to protect against control armyworm, stemborer, and/or termites.

2.2 The DayCent model

- 145 The DayCent model (version 2020 DayCent (2017 version of DD_EVI) is a terrestrial ecosystem model of intermediate com-plexity [\(Del Grosso et al., 2001\)](#page-52-1). It simulates *daily* C and N fluxes within the soil-plant-atmosphere continuum on a daily basis and has been parameterized for many several crops and ecosystems [\(Necpalova et al., 2018\)](#page-55-3). It has submodules to simulate plant growth, organic resource and soil organic matter (SOM) decomposition $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$ mineralization of N, soil water and temperature, N gas fluxes, and CH_4 oxidation. The net primary productivity of plants is a function of their ge-150 netic potential, a simplified phenology, solar radiation, temperature, and stresses, such as reduced water or N availability.
- Here, we used the non-growing degree day version of the DayCent crop module, which that does not simulate phenology but has a seedling stage with reduced growth until a certain biomass (full canopy) is reached. SOC and soil N in the upper 20 cm topsoil are represented by an active, slow, and passive SOM pools pool, while litter and organic resources are represented by a structural and metabolic litter pools pool [\(Parton et al., 1987\)](#page-55-4). All soil SOM pools are conceptual and
- 155 have no measurable counterparts, whereas the litter pools are semiquantitative, that is, their semi-quantitative. Their division is based on the measurable ratio of lignin to N in the organic resources and plant litter. For temperate conditions, DayCent has been shown to DayCent can adequately simulate crop yields, SOC and soil N dynamics, and N₂O emissions [\(Del Grosso et al., 2005;](#page-52-4) [Necpálová et al., 2015;](#page-55-1) [Necpalova et al., 2018;](#page-55-3) [Gurung et al., 2020,](#page-52-2) [2021\)](#page-53-2). Yet, for tropical conditions <mark>the performance has not been studied in similar detail. A</mark> in temperate conditions [\(Del Grosso et al., 2005;](#page-52-4) [Necpálová et al., 2015;](#page-55-1) Necpalov
- 160 but a recent paper showed that the general model fit of the uncalibrated model was suboptimal inadequate performance for tropical conditions [\(Nyawira et al., 2021\)](#page-55-2).

2.3 Data used for the DayCent model evaluation/calibration <u>and evaluation</u>

In a process that was repeated four times, a large data set was used based on

- To provide an overall assessment of the performance of DayCent for its use in Kenya a leave-one-site-out cross-validation 165 approach was applied. Specifically, this involved using a data sub-set from three of the four sites for the model calibrationand the validation was performed based on the model calibration, with validation performed using the data from the fourth site. The plot-scale yield of maize grain This process was repeated four times, every time with another site serving as the validation site. Different data, were used for this: Maize grain yield and the aboveground biomass, both on a dry matter basis(t ha⁻¹), were available for each cropping season between 2002 and 2020 (further details in [Laub et al., 2023b\)](#page-54-3). In addition to thatAll
- 170 this data was used with one exception the short rainy season of 2019 at Sidada, which had unrealistically high maize grain yields of up to 16 t ha⁻¹. In addition, plot-scale SOC and total N contents in the top 15 cm were available for several points over time soil layer were available at several time points, and in 2021 for the 0-30 cm soil depth. In Embu and Machanga, soil samples were taken every two to three years since initiation the start of the experiment in 2002 until 2021, but while in Sidada and Aludeka, <u>soil sampling occurred</u> only in 2005, 2018, 2019 and 2021 (further details in [Laub et al., 2022a\)](#page-53-1). Because
- 175 bulk density (further details in [Laub et al., 2023a\)](#page-54-4). Because soil bulk density data was not available for most soil samples and in 2021 -time points and there was no significant difference in topsoil bulk density between treatments at any site in 2021 , the mean soil bulk density per site was used to calculate SOC stocks of the top 15 cm of soil depth. All simulations were conducted at the site scale, so the plot-scale (i.e. replicate)measurements were aggregated to the site scale, calculating means and variances. DayCent calculates SOC to a depth of 20 cm , so we rescaled the SOC We used a DayCent parameterization that was developed
- 180 to simulate SOC stocks of the IPCC-recommended 0-30 cm topsoil layer [\(Gurung et al., 2020\)](#page-52-2) (further details in section [2.3.2\)](#page-8-0). Thus, the 0-15 cm SOC stocks were adjusted to 0-30 cm depth. This was done by adding the site-specific SOC stocks from the 15-30 cm layer (specifically, the 15-30 cm equivalent-soil-mass-based ones [\(Wendt and Hauser, 2013;](#page-57-2) [Lee et al., 2009\)](#page-54-6)) to the treatment-specific SOC stocks for the top 15 cm to the top 20 cm , using the formula of [Jobbágy and Jackson](#page-53-3) [\(2000\)](#page-53-3):

$$
SOC_{20}(kg \ ha^{-1}) = \frac{1 - \beta^{20}}{1 - \beta^{15}} * SOC_{15}
$$

185 Here, SOC $_{20}$ and SOC₁₅ are SOC stocks in kg ha⁻¹ in the top 20 and 15 from 0-15 cm. Due to limited data availability for the 15-30 cm soil depth , respectively. The parameter β is the relative decrease of SOC stocks with depth, for which we took

the mean values across sites (0.9725), calculated from the (only 2021 sampling, where samples from 0-15,), this approach was considered the most conservative and robust; subsoil carbon usually changes very slowly, and a statistical test revealed no differences in the equivalent soil mass based SOC stocks of the 15-30 , and 30-50 cm were available for all of the sites. cm layer (2.5-4.7 t soil ha⁻¹) between treatments at the same site in 2021 (with only one single exception in Aludeka; Fig. [A2\)](#page-42-0).

Data on N_2O emissions were used in the model evaluation phase, but not for model calibration, because the data were scarce and subject to high variability due to their scarcity and high uncertainty. The N_2O measurements were conducted after N fertilization in 2005 (weekly measurements form March to June in Embu and Machanga and daily measurements in Machanga in November), in 2013 and 2018 (weekly measurements form March to beginning of May in Sidada and Aludeka),

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- 195 and in 2021 (weekly measurements form mid-March to mid-May in Sidada). They were conducted with The measurements applied the static chamber method [\(Hutchinson and Mosier, 1981\)](#page-53-4) . Measuring frames were permanently installed in the plots with two measuring frames per plot permanently installed for a whole rainy season . The (one within, one between $_{\text{maxize rows}}$). The sampling chambers (0.27 \times 0.375 \times 0.11 m) were made of polyvinylchloride and equipped with had a vent tube and a fan to homogenize gas inside them before gas sampling. The measured N_2O emissions were evaluated at
- 200 two levels of aggregation. First, as site means per measurement day (from the three replicates, similar to all other data) fan for to homogenize the gas sample before extraction with a 60 mL polypropylene syringe through a septum-sealed sampling port. Four gas samples were collected at 0, 15, 30 and second as cumulative emissions over the whole season, for which we first 45 min of chamber closure. Gas samples from within and between maize rows were combined per time point in the same syringe [\(Arias-Navarro et al., 2017\)](#page-51-4). All analyses were conducted using a SRI 8610C gas chromatography (456-GC,
- 205 Scion Instruments, Livingston, United Kingdom) equipped with an electron capture detector for N₂O analysis. Fluxes per surface area were determined using the linear slope of gas concentration over time [\(Pelster et al., 2017;](#page-55-5) [Barthel et al., 2022\)](#page-51-5). $\text{Simulated N}_2\text{O emissions}$ were evaluated against measured daily and cumulative N_2O emissions. To determine the cumulative emissions at plot scale, we used the trapezoid method at the plot scale [\(Levy et al., 2017\)](#page-54-7), specifically, the trapz function of R [\(Tuszynski, 2021\)](#page-56-3). Site-scale Treatment-scale means and variances were then computed for these of the daily and cumulative
- 210 N_2 O emissions , similar to all were then computed in a similar way as for the other measurements. Furthermore, data on soil mineral N (N_{min}), measured as NH₄⁺ and NO₃⁻, and measured moisture content at soil depths of 0-15 cm, were available from several measurement campaigns in the years 2012, 2013, 2018, 2019 and 2020. Finally, in the control and the 1.2 t C plots of the *Calliandra*, farmyard manure and maize stover treatments, Finally, continuous soil moisture measurements from were conducted using sensors placed in each replicate at 10 cm soil depth (EC-5 Soil Moisture
- 215 Sensor, Meter, Germany) , were available for in the control and the 1.2 t C plots of the *Calliandra*, farmyard manure and maize stover treatments at the Sidada and Aludeka sites (March 2018 to December 2020). These soil moisture measurements data were used to initially determine the optimal pedotransfer functions for soil hydraulic conductivity before the actual model ealibrationphasebut not used in the model calibration.

2.3.1 Model driving variables and model assumptions

- 220 The site-specific crop management data used to run the DayCent model was obtained from field management operation records for each season at each site. This included specific dates for the yearly application of organic resources (in all but the control plots)season- and site-specific records of field management operations. These included dates of organic resource application, manual plowing before planting, maize planting, split application of mineral Nat rates of 40 kg and 80 kg N ha⁻¹ per season, weeding and harvestdates. Pesticide application events Dates of pesticide applications and gap filling plus maize thinning or
- 225 maize thinning were also available, but these operations are not part of standard DayCent management and were therefore not included in the DayCent schedule file. Our model runs therefore, modelling. Therefore, our model runs assumed no occurrence of pests or diseases, and an optimal plant density from the start, whichin practice at emergence, which, in practice, was ensured by manual thinning and gap filling.

The climate data used to run DayCent consisted of recorded data at each of the sites. However, filling the Recorded weather

- 230 data existed for all sites, but filling in data gaps was necessary due to unavailability and loss of recorded data. In At Embu and Machanga, manual recordings of daily minimum and maximum temperature and precipitation were available from 2002 until the end of 2007, but from 2008 until 2017, only measured precipitation was available. After 2017, high-quality data from newly installed TAHMO stations [\(https://tahmo.org/climate-data/\)](https://tahmo.org/climate-data/) were available near the Machanga and Embu sites, with for these two sites, providing daily values for temperature and precipitation. In Aludeka and Sidada, manual recordings
- 235 of daily minimum and maximum temperature and precipitation were available for all years from 2005 to 2017, during which high-quality weather stations were installed 2017. Thereafter, weather stations (Meter climate station, Meter Environment, Munich, Germany) <u>were installed and provided the dat</u>a. These data Data gaps were filled by using the NASA POWER product [\(https://power.larc.nasa.gov/docs/methodology/\)](https://power.larc.nasa.gov/docs/methodology/). A bias correction for the minimum and maximum temperature of NASA POWER data was performed, using a linear regression with measured data as dependent variable (y) and NASA POWER data
- 240 as independent variable (x). Specifically, the slope and intercept of the regression equation $y = mx + b$, were used to produce a corrected estimate of these data. In our specific case, the slopes were not significantly different from 1, but intercepts (b) were significantly different from 0. The specific intercepts for maximum temperature were -0.3 $^{\circ}$ C, -0.4 $^{\circ}$ C, +3 $^{\circ}$ C and +6 $^{\circ}$ C for Embu, Machanga, Sidada and Aludeka, respectively. The intercepts for the minimum temperature were -0.25°C, -0.5°C, -3°C and +1°C for Embu, Machanga, Sidada, and Aludeka, respectively. For precipitation, no bias correction was done.
- 245 The data on the hydraulic properties of the soil soil hydraulic properties needed in DayCent (volumetric soil water content at field capacity, wilting point, and saturated hydraulic conductivity K_s) were calculated based on the soil texture measured at each site. We tested two pedotransfer functions to see which one provided a better fit: (1) the widely applied function of [Saxton and Rawls](#page-56-4) [\(2006\)](#page-56-4) and (2) the function of [Hodnett and Tomasella](#page-53-5) [\(2002\)](#page-53-5) , which The pedotransfer functions of [Hodnett and Tomasella](#page-53-5) [\(2002\)](#page-53-5) was used, because it was specifically designed for tropical soils. Within the Hodnett and Tomasella (2002)
- 250 equationIts' soil hydraulic properties also showed better agreement between the measured and simulated soil moisture contents than when soil hydraulic properties of [Saxton and Rawls](#page-56-4) [\(2006\)](#page-56-4) were used. Because the [Hodnett and Tomasella](#page-53-5) [\(2002\)](#page-53-5) equation does not provide a method to estimate K_s , K_s was calculated using the [Saxton and Rawls](#page-56-4) [\(2006\)](#page-56-4) equation, with values of the

water retention curve, α and *n* [\(van Genuchten, 1982\)](#page-56-5), taken from [Hodnett and Tomasella](#page-53-5) [\(2002\)](#page-53-5), because their equation does not provide a way to estimate K_s. In initial test simulations, we compared the observed versus soil moisture contents in the top

255 15 cm, for which continuous measurements were available from Sidada and Aludeka from 2018 to 2020. In this comparison, the pedotransfer functions of [Hodnett and Tomasella](#page-53-5) [\(2002\)](#page-53-5)showed better agreement between the measured and simulated soil moisture contents than [Saxton and Rawls](#page-56-4) [\(2006\)](#page-56-4) and were consequently used in the application of the model at the four LTE sites calculated with the equation from [Hodnett and Tomasella](#page-53-5) [\(2002\)](#page-53-5).

2.3.2 Initial model parameterization and selection of potentially sensitive parameters for calibration

- 260 To parameterize the organic inputs, the mean lignin content and C/N ratio of the different organic materials across sites (Table [A2\)](#page-39-0) were used. This was justified approach was used because measurements were not available for all sites and yearsand because , and was justified as an analysis of variance of data from the years 2002, 2003, 2004, 2005 and 2006 for at Embu and Machangaand from the year , and from 2018 for all sitesat all sites, did not indicate any significant differences in lignin contents and C/N ratios between the sites or years. The C content $\frac{\text{in } \text{ of}}{\text{max}}$ grain was assumed to be 42.5% throughout the simulation 265 period. This was the mean value of measured grain C content across sites (standard deviation 1.8%), which were available
- from in the short rainy season 2018 and long rainy season 2019 (data not shown). Given the strong correlation between maize grain yield and above ground biomass $(r = 0.87)$, the above ground biomass data was transformed to harvest index data for the model calibration process, because harvest index had a lower correlation with yield $(r = 0.59)$ than aboveground biomass.

The DayCent simulations were conducted at the site scale using averaged treatment scale using average values across all three

- 270 graplicate plots for soil texture and parameters (i.e., soil texture, bulk density, pH), SOC and soil N stocks, <u>maize grain</u> yield and aboveground biomass. This /harvest index. This aggregation was done to reduce the computation time of the sensitivity analysis and calibration. Additionally, initial tests with the default DayCent parameterization showed that simulations and because initial tests showed similar model performance as compared to applying the model to each experimental replicate individually did not lead to better agreement between measured and simulated values than a single simulation of the average soil parameters of
- 275 the three replicates. Therefore, final model simulations were conducted with averaged values for soil parameters (i.e., texture, bulk density, soil pH) across the three replicates per site. For data used in model calibration and evaluation, the χ The sitespecific variance standard deviation for each type of measurement was used as a measure of uncertainty of the measured data (specifically, the median variance per site and measurement type computed from the three replicates from at each time point of each treatment). Site-specific variances were used because a statistical analysis of the data in earlier work had shown that
- 280 variance heterogeneity existed only between sites , for each treatment at each site). This choice was based on the statistical models of [Laub et al.](#page-54-4) [\(2023a,](#page-54-4) [b\)](#page-54-3), showing variance heterogeneity between sites but not between treatmentsat the same site [\(Laub et al., 2022a,](#page-53-1) [2023b\)](#page-54-3).

The standard parameter values of the DayCent 2020 version were taken as initial model parameters. The exceptionswere the decomposition parameters , with three exceptions. First, we used the adjusted decomposition parameter values of the

285 SOM pools . For these, we used updated estimates from a recent Bayesian calibration [\(Gurung et al., 2020\)](#page-52-2) that included data from most of the well-known long-term experiments in Europe and the US (and textures from 15-50% clay). To our knowledge [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2) provide the most up-to-date decomposition parameters, and hence, we assigned the median of reported parameter values for each SOM pool as initial parameter values in our model simulations. Furthermorefrom <u>[Gurung et al.](#page-52-2) [\(2020\)](#page-52-2) to allow the use of DayCent for simulating SOC stocks of the 0-30 cm soil depth layer instead of</u>

- 290 the standard 0-20 cm layer. Second, we modified the parameter value representing the fraction lost as CO₂ upon structural litter and lignin turnover (ps1co(1&2)&rsplig). The default value for this parameter is 0.5 assigning a carbon use efficiency <u>(CUE)</u> value of 50% to structural litter, based on outdated theories that lignin-rich materials form stable SOC most efficiently [\(Frimmel and Christman, 1988\)](#page-52-5). Newer studies have, however, clearly shown that minimal structural litter is conserved in the <u>long term, while metabolic litter forms SOC more efficiently [\(Cotrufo et al., 2013;](#page-52-6) [Denef et al., 2009;](#page-52-7) [Puttaso et al., 2013;](#page-55-6) Kallenbach et al.</u>
- 295 Thus, we opted for a more realistic prior value of 0.85 for ps1co(1&2)&rsplig, corresponding to a more plausible CUE value of 15% for structural litter [\(Mueller et al., 1997\)](#page-55-7). Third, for the parameters determining the minimum and maximum proportion [o](#page-53-2)f nitrified N lost as N₂O, we used the most values that fell between the DayCent default values and recent values from [Gurung](#page-53-2) [et al.](#page-53-2) [\(2021\)](#page-53-2), who showed that older parameters overestimate N₂O emissions. This choice was motivated by the fact that the DayCent default parameter values led to excessively high emissions, while the [Gurung et al.](#page-53-2) [\(2021\)](#page-53-2) parameter values resulted 300 in emissions that were too low. Finally, we assumed that the maize growth parameters of the second highest production level
	- (C5 in DayCent) represent best the production levels observed in the experiment.

To identify which model parameters to include in the global sensitivity analysis (see section [2.4\)](#page-11-0) and in the model calibra-tion, we screened the reviewed literature for recently conducted sensitivity analyzes of the DayCent model [\(Necpálová et al.,](#page-55-1) [2015;](#page-55-1) [Gurung et al., 2020\)](#page-52-2)and additionally used Additionally, we consulted the DayCent manual to identify and add further

- 305 parameters of potential importance for the processes considered in our study (i.e., plant productivity and soil C and N eveletime cycling). This resulted in a selection of 66 parameters (Table [1](#page-13-0) and Table [A3\)](#page-40-0). Some of these parameters represented groups of the same type of parameters that can each belong to the same category, but can be individually calibrated in DayCent, e. g., For example, the "tillage multiplier" of SOM turnover can have different values for different SOM pools . However, because the tillage multipliers are but is usually the same for all SOM pools in the standard DayCent parameterization. Thus, we decided
- 310 to have the same tillage multiplier value for active, slow, all SOM and litter pools. In addition, some of the Some parameters can have different values between the SOM pools of the surface and soil (for exampleSOM pools (e.g., C/N ratios and turnover rates). For simplicity, we decided to assign ass<u>igned</u> the same C/N ratios and a constant ratio to the turnover <u>rates</u> of surface and soil SOM pools . Because the turnover rates of the SOM pools are typically faster on the surface than in the soil, we defined a new parameter that represents the value ratio of the surface to the soil parameters (i.e., $decX(2)/decX(1)$). This allowed us
- 315 to jointly evaluate the sensitivity and calibrate parameters related simplified parameter sensitivity analysis and calibration with regard to surface and soil SOM poolswithout adding too much complexity. Finally, the parameters for governing the minimum and maximum values of nitrification and loss of nitrified N as N₂O, were reformulatedas maximum and the were reformulated. Instead of calibrating them as a maximum and a minimum value, we considered the maximum value and the difference between the minimum and maximum parameters values (i.e., N2Oadjust_(max-min) and aneref(1)-anaref(2)). This was done to ensure
- 320 that the maximum was always higher than the minimum valuein order to avoid numerical problemsensured that the minimum

value was smaller than the maximum value, thereby avoiding numerical problems(initial N2Oadjust_max was set to 0.015; N2Oadjust_(max-min) to 0.003).

2.3.3 Spin-up and site history simulation to initialize SOC and soil N contents Soil organic matter pools initialization <u>based on measured data</u>

- 325 As is standard practice in DayCent, the initialization of SOM pools was conducted through a Instead of relying on spinup run, which was followed by a simulation of the history of the site before experiment establishment based on simulation based on uncertain historical land use and management of the simulated sites, we used measured mineral associated organic ✿✿✿✿✿ carbon (MAOC) fractions as a proxy for the initialization of the knowledge of site managers. The spin-up has the aim to initialize the SOM pools to equilibrium using the typical input of biomass of the native vegetation type. The type of native
- 330 vegetation for each site was determined from an available potential vegetation map [\(Kamoni et al., 2007\)](#page-53-0) and confirmed by site managers as tropical evergreen forest in Embu, dry savanna in passive SOM pool [\(Zimmermann et al., 2007\)](#page-57-3). Replacing SOM initialization assumptions with measured proxies can enhance model performance [\(Laub et al., 2020;](#page-53-7) [Wang et al., 2023\)](#page-57-4) , and, more importantly, is less sensitive to user assumptions. It also aligns with the DayCent concepts on SOM; the manual [\(Hartman et al., 2020\)](#page-53-8) denotes that particulate organic carbon (POC) and MAOC are related to the slow and the passive SOM
- 335 pool, respectively. MAOC data for samples from the 0-30 cm soil layer was available from the year 2021 (specifically for the control -N, control +N and the farmyard manure -N and Tithonia diversifolio -N treatments at 4 t C ha⁻¹ yr⁻¹ at all sites). It was derived by density fractionation using sodium polytungstate solution (1.6 g cm⁻³ for Aludeka and 1.7 g cm⁻³ for the other sites). Aggregates were dispersed with ultrasonication at 400 J ml⁻¹ (217 s at 200-240W), after which samples were centrifuged for 2h at 4700 rpm to separate the heavy and the light fraction, which were then separated, washed with deionised water, dried
- 340 at 60 °C for 24h and analyzed for weight and C content. A statistical analysis revealed the absence of treatments differences within the same site, so the site-specific MAOC values for the 0-30 cm soil depth across treatments (0.91, 0.88, 0.85, 0.86 g MAOC g⁻¹ SOC for Aludeka, Embu, Machanga, and humid savanna in Sidada and Aludeka. A 2000-year spin-up simulation was sufficient to reach a steady state of SOM pools. Site managers had a good knowledge of the type of historical cropping systems, e. g., arable vs. grasslands, types of crop rotation (e.g., maize monoculture vs. crop rotation with legumes), manure
- 345 inputs and management, but without detailed information on the duration of these systems. Therefore, the duration of cropping systems after native vegetation was adjusted at each site so that Sidada in 0-30 cm, respectively) were used to initialize the SOC in the passive SOM pool in DayCent simulations. Further, 3% of initial SOC was assigned to the active SOM pool (mean value recommended in the DayCent manual) and the remainder of SOC was assigned to the slow SOM pool.
- The DayCent manual further states that, although the slow SOM pool is closely related to the POC fraction, it tends to be 350 larger [\(Hartman et al., 2020\)](#page-53-8). Consequently, the passive SOM pool must be smaller than the MAOC fraction. Additionally, the fractionation data was from 2021, when the experiments were already 19 and 16 years old. To address these issues, two new parameters were introduced in the simulations: 1) an intercept (IC_{MAOC}) to account for the passive SOM pool being smaller than the MAOC fraction, and 2) a slope for the time since the start of the experiment (SL_1) to account for SOM changes (mostly losses) since the start of the experiments, with the passive SOM pool typically changing at the slowest rate.

355 Given that all sites were converted to agriculture only a few decades ago [\(Laub et al., 2023a\)](#page-54-4), the percentage of total C in the passive SOM pool at the start of the experiment should be higher than the 30-40 %, that are common at steady state of SOM pools [\(Hartman et al., 2020\)](#page-53-8). Considering this, it was assumed that the intercepts initial value was -0.1 g MAOC g⁻¹ SOC and the slopes initial value value was -0.005 g MAOC g⁻¹ SOC yr⁻¹ since the measured initial SOC stocks corresponded to the simulated SOC stocks at the start of the experiment. Additionally, to achieve suitable levels of soil N stocks after the spin-up. **the maximum C/N ratio of**, giving both terms approximately the same weight. Thus, the fraction of SOC in the passive SOM

pool at the start of the experiment was

$SOC_p(g\ g^{-1}) = MAOC_{2021} + IC_{MAOC} + SL_t * t_{dif}$ ✿✿

(1)

Here, $\mathrm{SOC_{p}}$ represents the fraction of $\mathrm{SOC_{m}}$ the SOM pools had to be increased. It was increased from 14 to 20 for the active SOM pool and from 8 to 13 for the passive SOM pool (parameters varat12&11(1, 1)and varat3(1at the start of the experiment, 365 MAOC₂₀₂₁ the MAOC fraction in 2021 (g MAOC g⁻¹ SOC), IC_{MAOC} the intercept, and SL_t the slope value that is multiplied by the time difference between the measurement and the start of the experiment in years (t_{dif}). With the selected standard values for IC_{MAOC} and SL_t, between 66% (Machanga) and 73% (Aludeka) of SOC were assumed to be in the passive SOM pool at the start of the experiment. The uncertainty related to this initialization approach was accounted for in the model calibration by allowing large ranges for these parameters. Finally, to initialize the soil N pools, C/N ratios of the active, slow, and passive

370 SOM pools were set to 10, 1), respectively). Due to computational time constraints and to ensure a match between simulated and observed initial SOC and soil N levels, the spin-up and site history simulations were not included in the sensitivity analysis and Bayesian calibration 17.5, and 8.5, respectively, which are the best estimates provided by the manual [\(Hartman et al., 2020\)](#page-53-8)

2.4 Global sensitivity analysis

.

- 375 To reduce the dimensionality of the calibration of the modelnumber of optimised parameters during the calibration, we performed a parameter screening [\(van Oijen, 2020\)](#page-56-6). For this purpose, a global sensitivity analysis was conducted to quantify the relative importance of different model parameters to the relevant model outputs regarding our study<u>'s</u> focus on maize yield and $\overline{\text{IFM}}$ the greenhouse gas mitigation potential . The goal was to of ISFM. The aim was to identify and fix less influential model parameters to their default initial values, reducing the computational cost for performing the consecutive Bayesian model cal-
- 380 ibration (see section [2.5\)](#page-12-0). Global The global sensitivity analysis was performed using the Sobol method [\(Saltelli, 2002a,](#page-56-7) [b\)](#page-56-8), which allows for the estimation of the proportion of variance in the model outputs that is explained by each model parameter, while considering the interaction terms of first-order and higher-order [\(Gurung et al., 2020\)](#page-52-2). The "sensitivity" package (function sobolSalt; [Iooss et al., 2021\)](#page-53-9) of R version 4.0 [\(R Core Team, 2020\)](#page-55-8) was applied. This function implements a simultaneous Monte Carlo estimation of first-order and total-effect Sobol indices. The computational cost is $N(p+2)$ model runs, N being
- 385 the dimension of the two matrices to construct the Sobol sequence, p being the number of parameters (66 in our case). Our tests indicated similar results for $N = 500/1000$, so we chose a dimension of 1000. The preselection of preselected model

parameters to include (are described above and in Tables [1](#page-13-0) and A3) is described above. Independent uniform prior distributions were used for the global sensitivity analysis, with the upper and lower parameter boundaries centered around the default initial parameter value obtained as described belowabove (section [2.3.2\)](#page-8-0). We based the global sensitivity analysis parameter ranges

390 on previous sensitivity analyses (e.g. [Necpálová et al., 2015;](#page-55-1) [Gurung et al., 2020\)](#page-52-2), θ -plausible ranges reported in the DayCent manual and on how the parameters varied between variations observed in different maize parameterizations in the literature. The parameters were then grouped by how large the ranges were. The parameters that had according to the magnitude of their ranges. Parameters with very small, small and moderate ranges were varied by ± 10 , 25 and 50% from the default initial parameter value, respectively. For parameters with large and very large ranges, the upper/lower boundaries were the default 395 initial parameter values multiplied/divided by 3 and 10, respectively. Additionally, we assumed that the maize parameters of the second highest production level (C5 in DayCent) would best represent the production levels in the experiment. The parameter sensitivity was independently determined for the mean maize grain yield , and aboveground biomass, averaged over all seasons at all sites, as well as for the SOC and soil N stocks at the end of the simulation period.

2.5 Combined Bayesian calibration of plant and soil model parameters

400 Joint Bayesian calibration of the sensitive DayCent parameters was performed using all available data on maize grain yield, aboveground biomass,and SOC stocks. The main reason for only using these data was that the yields, SOC stocks, and their trade-offs were the focus of this study. A second, technical reason, was that the creation and readout of daily simulations outputs, needed to match simulated and measured soil moisture content, mineral N content and

2.5 Combined Bayesian calibration of plant and soil model parameters

405 Bayesian calibration is a probabilistic inverse modeling $\frac{1}{2}$ data assimilation technique, which is used to estimate the joint posterior distribution of model parameters (θ) given the measured data (D) and the model structure (M), expressed as $p(\theta|D,M)$. It uses the proportionality form of Bayes' theorem, where $p(\theta|D, M)$ is proportional to the prior belief about model parameters, $p(\theta)$ times the likelihood function $\frac{1}{r}p(D,M|\theta)$: of the data given the model and the parameters, $p(D|M,\theta)$:

$$
p(\theta|D,M) \propto p(\theta) * p(D,M|M,\theta) \tag{2}
$$

- 410 While the prior, $p(\theta)$, is chosen based on previous knowledge of the model parameters, the likelihood function, $p(D, M | \theta)p(D|M, \theta)$, measures how well the model and the data match. In practice it is derived for a given set of parameter parameters sampled from the prior, by running and evaluating the model using the measured data, the simulated counterpart and the variancecovariance matrix of the data. We used the median variances per site for each type of measurement (computed from the three replicates) as the diagonal elements of the variance-covariance matrix. Due to the large number of observations and the mostly
- 415 **balanced dataset, the off-diagonal elements were set to 0.** model residuals. Following [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2), we applied the R software [\(R Core Team, 2020\)](#page-55-8) to create a mixed model with restricted maximum likelihood estimation with the lme4 package

Table 1. DayCent model parameters and the coefficient of variation used in the calibration. Displayed are parameters considered for calibration due to total sensitivity index > 2.5% (top) and with a total sensitivity index > 1% (bottom). The remainder of parameters (51%) can be found in the supplementary (Table [A3\)](#page-40-0).

tedes to microbial carbon use efficiency); thighest likelihood parameter set across all four sites

[\(Bates et al., 2015\)](#page-51-6), which automatically constructed the variance covariance matrix based on the nested design of observations to account for autocorrelation of residuals. The likelihood was a function of the following form:

$$
p(D|M,\theta_z) = \frac{1}{\sqrt{2\pi\Sigma}} \exp\left(-\frac{1}{2}(M(\theta_z) - D)^T \Sigma^{-1}(M(\theta_z) - D)\right)
$$
(3)

420 Here, Σ is the variance covariance matrix, $M(\theta_z)$ is the vector of simulated values using the z-th parameter set θ_z and D the vector of observed data. In the R software, this can be constructed by setting the residual (modelled value - measured) as the dependent variable of a zero intercept model with nested random effects (i.e., sampling date within site), and assigning the inverse of the median standard deviation (of each type of measurement at each site) as weight. The logLik() function is then used to extract the log-likelihood, which is transformed to the likelihood by raising e to the power of the log-likelihood.

425 The sampling importance resampling method, which was used in this study, is a direct form of Bayesian calibration, which has recently been used by [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2), to calibrate the parameters of the SOM module of DayCent using a large collection of temperate long-term experiments. It samples the prior by running the model for a large sample of parameter sets of size *I* from the prior, computing the likelihood for each sample, and filtering the prior based on importance weights $w(\theta_z)$

$$
w(\theta_z) = \frac{p(D, M|\theta_z)}{\sum_{i=1}^{I} p(D, M|\theta_i)} \frac{p(D|M, \theta_z)}{\sum_{i=1}^{I} p(D|M, \theta_z)}
$$
(4)

430 where $p(D, M | \theta_z)$ $p(D|M, \theta_z)$ is the likelihood function of the *z*th parameter set and $w(\theta_z)$ is the corresponding importance weight. It is consistent with the proportionality form of Bayes' theorem in that it uses the importance weights $w(\theta_z)$ as probabilities for sampling from the prior, without replacement, to derive the posterior.

Combined Bayesian calibration of the sensitive DayCent parameters was performed using all available data on maize grain yield, harvest index (calculated from aboveground biomass), and SOC stocks. A notable exception was that SOC stocks

- 435 from the Machanga site were not used in the calibration process, because this site was severely affected by soil erosion [\(Laub et al., 2023a\)](#page-54-4) that is not represented by DayCent. The main reason for only using grain yield, harvest index and SOC data was that the yields, SOC stocks, and their trade-offs were the focus of this study. Technical constraints also influenced the decision; the creation and readout of daily simulation outputs to match simulated and measured soil moisture content, mineral N content and N₂O fluxes would slow down the whole Bayesian calibration process by a factor of 5. The Bayesian
- 440 calibration would have taken more than three months on the virtual machine with 64 cores. Following [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2) model parameters that had a total sensitivity index of at least 2.5% for either yield, aboveground biomass, or SOC were considered influential and thus were subjected to calibration (11 parameters). Additionally, the new parameters associated with the initialization, IC_{MAOC} and SL_t had to be calibrated, resulting in a total of 13 parameters for calibration (Table [1\)](#page-13-0).

Overall, a total of 200000 simulations were performed, from which $\frac{1}{x}$ as in 0.1% (200) of the parameter sets were sampled 445 to derive the posterior distribution through resampling [\(Gurung et al., 2020\)](#page-52-2). It was assured that this number of simulations was sufficient by splitting the simulations into two halves and visually assessing the similarity of derived posteriors for these subsets. In our experience, the sampling importance resampling algorithm is ideal-highly suitable for DayCent, which that is prone to model crash when using crashing with inappropriate parameter combinations. This method does not depend on chains, but rather on Unlike chain-dependent methods such as Markov Chain Monte Carlo, this method relies on model runs

450 that are independent of each other. This means_s, ensuring that an erroneous run does not stop the algorithm, as would be the case in chain-dependent methods such as Markov chain Monte Carlo. In addition, this strategy method allows for an efficient cross-validation of the posterior parameter set.

To evaluate the model by comparing measured vs. modeled data, we conducted a , such as the leave-one-site-out crossvalidation . This means that each of the sites is left out one by one for an independent evaluation, while the other three 455 sites were used to compute the resampling weights and derive the posterior parameter distributions. Hence, the evaluation is representative of up-scaling exercises of the DayCent model to other sites, because it involves evaluation of the model performance across different sites. Here, the SIR algorithm was also advantageous. We stored the model employed in this study. Notably, the sampling importance resampling algorithm's advantage lies in its ability to store model results for each parameter set by site, which meant that the allowing for straightforward cross-evaluation could be done by a simple filter by by

460 site, without <u>the need for</u> rerunning the model for each iteration. In contrast to model The posterior parameter distributions of this study are displayed for both the leave-one-site-out cross-validation , the parameter posterior distributions are not displayed by site. They are displayed for all four combined sites ; hence the full dataset without leaving any site out was used to derive them. This was done to present the and the combined dataset from all four sites (Fig. [2\)](#page-19-0). The former shows the importance of individual sites in the calibration process, while the latter provides the most representative posterior distributions and to make

465 distribution for model upscaling, making efficient use of all available data.

To ensure computational efficiency, we used informed Gaussian priors that were centered around the standard parameter values of DayCent, with coefficients of variation of 0.05, 0.1, 0.15, 0.25 and 0.3 for parameters with very small, small, moderate, large and very large ranges (Table [1\)](#page-13-0). For the newly introduced parameters, we used larger coefficients of variation, namely 1 for IC_{MAOC} and 0.35 for SL₁. Additionally, all parameters were constrained to remain within their physically sensible limits (i.e., not <0 for all and not >1 for those representing fractions).

2.6 Model evaluation

470

We used the following standard model evaluation statistics [\(Loague and Green, 1991\)](#page-54-8):

$$
MSE_y = \frac{1}{n} \sum_{z=1}^{n} (O_{yz} - P_{yz})^2
$$
\n(5)

$$
RMSE_y = \sqrt{MSE_y} \tag{6}
$$

475
$$
EF_y = 1 - \frac{\sum_{z=1}^{n} (O_{yz} - P_{yz})^2}{\sum_{z=1}^{n} (O_{yz} - O_y)^2}
$$
 (7)

Here, π the *MSE_y* is the mean-squared-error and *RMSE* is its root. EF_y is the Nash-Sutcliffe modeling efficiency. θ_{yz} is the measured value of the *z-th* measurement of the *y-th* type of measurement, \bar{O}_y the mean of the *y-th* type of measurement and $P_{\overline{y}}$ the simulated value corresponding to $O_{\overline{y}}$. We further divided MSE_y into squared bias (*SB*), nonunity slope (*NU*) and lack of correlation (*LC*), as suggested by [Gauch et al.](#page-52-8) [\(2003\)](#page-52-8). We expressed them as a percentage of the *MSEy*:

$$
480 \tSB_y(\%) = \frac{(\bar{O}_y - \bar{P}_y)^2}{MSE_y} * 100 \t(8)
$$

$$
NU_y(\%) = \frac{(1 - b_y)^2 * (\frac{\sum_{z=1}^n (O_{yz}^2)}{n})}{MSE_y} * 100
$$
\n(9)

$$
LC_y(\%) = \frac{(1 - r_y)^2 \cdot (\frac{\sum_{z=1}^n (P_{yz}^2)}{n})}{MSE_y} \cdot 100
$$
\n(10)

Here, Q_{yz} is the measured value of the z-th measurement of the y-th type of measurement, \overline{Q}_x the mean of the y-th type of measurement and P_{yz} the simulated value corresponding to Q_{yz} . \bar{P}_y is the mean predicted value of the *y-th* measurement type, 485 *b* the slope of the regression of *P* on *O* and *r* the correlation coefficient between *O* and *P*. The indicators *LC*, *SB* and *NU* show the nature of model errors, that is, a high *LC* shows that it is mostly random, a high *SB* a systematic bias, while a high *NU*

shows issues of model sensitivity.

2.7 Net global warming potentialGreenhouse gas balance

To compare different ISFM treatments in terms of their greenhouse gas (GHG) emissions, their net global warming potential 490 (GWP) GHG balance was computed on a yearly basis (kg CO₂eq ha⁻¹ yr⁻¹) was derived from the outputs over the whole simulation period. It was calculated from This calculation was based changes in the SOC content and cumulative emissions of $\rm N_2O$ using a 100-year time horizon of global warming potentials [\(Necpalova et al., 2018\)](#page-55-3):

$$
\underline{GWPGHGbalance} = \frac{44}{12} * \Delta SOC + 265 * N_2O \tag{11}
$$

Here, \triangle SOC is the change in SOC content (kg C ha⁻¹ yr⁻¹), N₂O the cumulative N₂O flux (kg N₂O ha⁻¹ yr⁻¹). The CH₄ 495 oxidation capacity was not considered, because it usually makes a very limited contribution to GWP in rainfed maize eropping systems GHG balance in rainfed cropping systems [\(Lee et al., 2020\)](#page-54-1) and we did not have data to evaluate the reliability of this simulated flux. In addition to GWP we calculated the net annual GHG balance, we calculated the yield-scaled GWP GHG b alance (in CO₂eq kg⁻¹ maize grain yield) by dividing the cumulative $GWPQHG$ balance over the entire simulation period by cumulative simulated yields (dry matter base).

500 3 Results

3.1 Most sensitive DayCent parameters

The results of the global sensitivity analysis showed that of the 66 model parameters includedanalyzed, only 20 parameters had a Sobol total sensitivity index >1% for either maize grain yield, aboveground biomass, SOC or soil N stocks (Fig. [1\)](#page-17-0). Of these, only 11 parameters had a Sobol total sensitivity index >2.5%, a threshold that captures the most influential parameters 505 and represents a suitable selection of parameters for model calibration [\(Gurung et al., 2020\)](#page-52-2). The parameters that turned out

Figure 1. Results of the uncertainty-based-global sensitivity analysis of the most relevant DayCent model parameters. Parameter sensitivity was independently determined for the mean maize aboveground biomass, grain yield, and SOC and soil N stocks at the end of the simulation period. Only parameters with a Sobol sensitivity index >1% are displayed.

to be the most sensitive, with a Sobol total sensitivity index $>10\%$ for at least one type of measurement, were radiation use efficiency ($prdx(1)$; for all measurement types); the optimal and maximum temperature for maize growth ($ppdf(1)$ and $ppdf(2)$, respectively; only for grain yield of maize and aboveground biomass), and maximum harvest index (himax; only for <mark>erop grain</mark> yield). Further, the turnover rate of the slow and passive SOM pools (dec5(2) and dec4, respectively; only for SOC and soil N),

- 510 the decomposition multiplier after tillage events for <u>soil tillage</u> (clteff(1,2&4); only for SOC and soil N) and the fraction lost as CO₂ upon of the metabolic litter pool turnover (pmco2(1&2), i.e., 1 - microbial carbon use efficiency (CUE); only for SOC and soil N) belonged to the most sensitive model parameters. The parameters of further importance, with a Sobol total sensitivity index <10% and >2.5% and <10%, were the minimum value for the impact factor of anaerobic soil conditions (aneref(3); only for SOC and soil N), the scaling factor for potential evapotranspiration (fwloss(4); only for maize grain yield), and the fraction
- 515 lost as CO₂ upon of the structural litter and lignin turnover pools (ps1co(1&2)&respligrsplig, i.e., 1-CUE; only for SOC and soil N). The fact that the Sobol 1st order and total sensitivity indexes were similar for most parameters suggested only a limited number of interactions between the parameters identified by the global sensitivity analysis.

3.2 Posterior parameter distributions from the Bayesian model calibration

Following the global sensitivity analysis, 11 selected 13 selected model parameters were calibrated using Gaussian priors

- 520 centered around the initial parameter value, with standard deviations according to the uncertainty ranges (Table [1\)](#page-13-0). The ranges of the same ranges of possible values as defined for the sensitivity analysis. Four parameters were fully constrained by the Bayesian calibration, one was partly constrained and tended towards the upper boundary. Four showed a tendency, but values from the whole prior range were present in the posterior distribution. Finally, two showed almost no difference to the uniform prior distribution prior- and the posterior distributions, using data from all four sites, were similar. Also the four different
- 525 posterior distributions from the leave-one-site-out cross-validations were largely similar to each other (Fig. [2\)](#page-19-0). Very clearly constrained were the potential maximum maize production and the maximum maize harvest index (2.5 However, several parameters slightly shifted from their initial values to the best parameter values across all four sites. The strongest differences between the initial and calibrated values existed for the potential maximum maize productivity per radiation (prdx(1); from 2.25 $\rm \frac{1.85}$ g C m⁻² langley⁻¹ for prdx(1)and 0.48 g g⁻¹ for himax), with values slightly higher than the default values and somewhere
- 530 in between the maize with the highest and second highest production levels (default DayCent maize parameters,named C6 and C5). Furthermore,the scaling factor for potential evapotranspiration was clearly constrained and slightly higher than the default value (fwloss(4), 0.9 vs 0.75). The the parameter representing the increase of SOM turnover after tillage (clteff(1,2,&4); from 10 to 19.1). An increase of the turnover rate of the slow SOM pool was also clearly constrained, but was centered around a value twice the default $(0.2 \text{ vs } 0.1 \text{ passive } \text{SOM pool}$ (dec4; from 0.0035 to 0.0056 g g⁻¹ yr⁻¹for dee5(2)). The was partly
- 535 counterbalanced by a decrease in the turnover rate of the passive SOM pool was clearly constrained at the lower end of possible values, it was centered around a much higher value than the default value (0.03 vs 0.0035 g g⁻¹ yr⁻¹ for dec4) and tended towards the upper boundary. A test with even broader ranges (up to 0.1 slow SOM pool (dec5(2); from 0.10 to 0.06 g g⁻¹ yr⁻¹)showed that the value around 0.03 g g⁻¹ yr⁻¹ was in fact the center of the posterior distribution of this parameter (Fig. ??), but allowing the parameters to vary that much reduced the model performance to unfeasible levels (model output not shown). The optimal
- 540 production temperature for maize (ppdf(1)) tended to have values lower than the default value, while the opposite was true for the maximum production temperature (ppdf(2)). Also the parameters representing $CO₂$ loss upon turnover of metabolic and structural litter pools^{of}. Furthermore the loss of carbon from the metabolic litter pool upon decomposition was significantly increased (pmco2(1&2)and ps1co2(1&2)&rsplig) tended towards higher values than the default values of these parameters (i. e., lower carbon use efficiencies, because the parameters represent 1-CUE), but they were not clearly constrained. Finally, the
- 545 parameters representing the increase of the SOM pools turnover after tillage (clteff(1, 2, & 4)) and the maximum rate limitation of soil under anaerobic conditions (aneref(3)), were poorly constrained.

Only a few strong correlations existed between the parameters of the $\frac{1}{2}$ from 0.54 to 0.82 g g⁻¹). The two parameters that translated measured MAOC into SOC in the passive SOM pool were altered in opposite directions (IC_{MAOC}, from -0.1 to -0.21) $g g^{-1}$; and SL_4 , from -0.005 to -0.0024 $g g^{-1}$ yr⁻¹). Overall, the parameter correlations in the posterior parameter set (Fig. [A3\)](#page-43-0).

550 Namely, there was a strong positive correlation $(r = 0.63)$ between the potential maximum production of maize (prdx(1)) and the optimal temperature for maize growth (ppdf(1)), the latter also being positively correlated with the maximum temperature

Figure 2. Prior compared to the posterior model parameter distribution resulting from the uncertainty-based Bayesian model calibration of DayCent using data from all sites combined (top) and the leave-one-site-out cross-validation (bottom). Dashed vertical lines represent the values of the default initially selected parameter set. The posterior distributions are based on all four study sites combined. For the description of the parameters see Table [1.](#page-13-0)

for maize growth (ppdf(2); $r = 0.45$). Furthermore, there was a negative correlation ($r = -0.43$) between the effect of tillage on SOM turnover and the amount of $CO₂$ loss upon turnover of the metabolic litter pool (pmco2(1&2)). The other correlations of the parameters were weak (i.e., below \pm 0.4)and therefore were of low importance across the four sites were minimal, and in 555 no case stronger than 0.2 (Fig. [A3\)](#page-43-0).

3.3 Simulation of maize grain yields and aboveground biomass at harvest

Although While the overall variation of maize grain yields between across sites and treatments could be captured with the set of default model parameters, the comparison of model results obtained with the default parameters compared to the set of parameters chosen for each site by to some extent with the initial model parameter set, for two sites a negative model efficiency

Figure 3. Simulated compared to measured maize grain yields at the four study sites for the initial DayCent parameter set (top) versus the calibrated parameter set by leave-one-site-out cross-validation (bottom). The 2985 data points correspond to the observations from the experimental treatments over 32 to 38 seasons, depending on the site. Symbols represent the different organic resource and chemical nitrogen fertilizer treatments. Grey bands show the 95% confidence intervals of measured (horizontal) values and the 95% credibility intervals of posterior distribution (vertical). Abbreviations: EF, Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation. Across all sites model statistics: EF, 0.358; RSME, 1.757 t ha⁻¹; SB, 21%; NU, 1%; LC, 77% before and EF, 0.495; RSME, 1.558 t ha⁻¹; SB, 2%; NU, 5%; LC, 93% after calibration, with 54% of measurements being in the 95% credibility interval of the posterior.

Figure 4. Simulated compared to measured maize grain yields aboveground biomass (AGB) at the four study sites for the default initial DayCent parameter set (top-lefttop) versus the calibrated parameter set by leave-one-site-out cross-validation (top-rightbottom). The same is displayed for maize aboveground biomass (AGB), showing the default DayCent parameter set (bottom-left) versus the calibrated parameter set (bottom-right). The 2985 data points correspond to the observations from the experimental treatments over 32 to 38 seasons, depending on the site. Symbols represent the different organic resource and chemical nitrogen fertilizer treatments. Grey bands show the 95% confidence intervals of measured (horizontal) values and the 95% credibility intervals of posterior distribution (vertical). Abbreviations: EF, Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation. Across all sites model statistics: EF, 0.033; RSME, 4.392 t ha⁻¹; SB, 27%; NU, 1%; LC, 72% before and EF, 0.254; RSME, 3.856 t ha⁻¹; SB, 3%; NU, 12%; LC, 85% after calibration, with 51% of measurements being in the 95% credibility interval of the posterior.

- 560 was obtained (Fig. [3\)](#page-20-0). With the leave-one-site-out cross-validation showed that the Bayesian calibration significantly improved the fit of the model for both maize grain yield and aboveground biomass (Fig[.3\)](#page-20-0). The calibration improved approach, the model efficiency for maize grain yields at the left-out site improved ubiquitously (i.e., from 0.32 to 0.39 in Aludeka; from 0.04 to 0.16 in Embu; from 0.32 to 0.36 in Machanga, from -0.16 to 0.27 in Sidada, and from 0.36 to 0.50 across all sites and so did RSME and bias. The same was true for the simulation of grain yield for all sites and for aboveground biomass for
- 565 all sites except Machanga (Fig. ??). It should be noted that despite excluding the evaluation site in the calibration step, the calibrated model was unbiased and errors mostly random for both yield (i.e., lack of correlation (LC) increased from 90% to 97%) and aboveground biomass (LC increased from 71% (e.g., from 0.03 to 91%). 0.25 across sites; Fig. [4\)](#page-21-0), with the exception of Machanga. Overall, biases in simulated grain yields were mostly eliminated through the model calibration, and biases in simulated aboveground biomass were eliminated in Aludeka and Siadada, reduced in Embu, but increased in Machanga.
- 570 Furthermore, while DayCent was inclined to overestimate the lowest and underestimate the highest values of The simulated posterior credibility intervals of simulated yields and above ground biomass contained 50% and 51% of observed data, respectively, <u>showing a that it could not capture the full uncertainty of measurements. While DayCent could not capture the full season-to-season</u> variability of grain yields and aboveground biomass, the mean yields and aboveground biomass per treatment throughout the simulation period were simulated well for most treatments without the addition of mineral N (Fig. [A3\)](#page-44-0). The exception to this
- 575 was that the Embu site, where there was a systematic underestimation of yields in the -N treatments. Interestingly, DayCent poorly distinguished the mean yields and aboveground biomass of treatments with high compared to very high rates of N inputs (i.e., the differences between the different organic resources and the control within the $+N$ treatment). An additional test of the model sensitivity of mean yields to different levels of mineral N fertilizer in the control provided further insights into this (Fig. [A5\)](#page-45-0). In this test, the yields stopped increasing plateaued at mineral N rates that were lower than the maximum N rates
- 580 provided in the organic resource +N treatments by mineral N and organic resources combined (up to >500 kg N per year or > 250kg N per growing season). In Machanga and Embu, simulated mean yields stopped increasing at around 100 kg N ha⁻¹ per growing season, which is less the 120 kg N ha⁻¹ per season that growing season in the control +Nreceived. In Aludeka and Sidada, simulated mean yields stopped increasing at 200 to 250 kg N ha⁻¹ per $\frac{1}{2}$ per $\frac{1}{2}$ season, but most of the response to N was below 120 kg N ha⁻¹ per $\frac{1}{20}$ growing season (Fig. [A5\)](#page-45-0).
- 585 Although the mean yields of the high-quality inputs in the in -N treatments with the high-quality inputs were well simulated, some of the low-quality input treatments in Aludeka and Sidada, namely maize stover at 1.2 t C ha⁻¹ yr⁻¹, and sawdust at 1.2 and 4 t C ha⁻¹ yr⁻¹, had lower simulated $yields$ than the than observed mean yields in their -N treatments (Fig. [5\)](#page-23-0). The same was true for the control -N in Aludeka , but the yields for sawdust -N at 4 t C ha⁻¹ yr⁻¹ in Machangawere overpredicted compared to measurements. Interestingly, the 95% credibility intervals for yield and aboveground biomass produced by the 590 leave-one-site-out cross-validation contained only about 30% of measured data and also tended to be considerably smaller than
	- variance-based 95% confidence intervals for the measured data. and Machanga.

Figure 5. Barplots of mean simulated and mean measured maize grain yield and aboveground biomass (AGB) from cross-validation. Error bars represent standard deviation.

3.4 Simulated SOC stocks in response to integrated soil fertility management

In contrast to the simulation of maize grain yields, the simulations of change in SOC stocks following the application of organic resources at different rates $(1.2 \text{ and } 4 \text{ t} \text{ ha}^{-1} \text{ yr}^{-1})$ was poorly simulated by DayCent with the set of default parameters. The

- 595 simulated SOC losses were too low compared to were not generally improved across sites by the observations leave-one-site-out cross-validation approach compared to using the initial model parameter set (Fig. [6\)](#page-25-0). The posterior parameter set obtained through Bayesian calibration with strongly increased SOM turnover rates showed a tendency for a higher loss of CO₂ from the turnover of metabolic and structural litter pools. With the posterior parameter set , Both the initial parameter set and the model, in calibrated parameter set resulted, however, in a better model performance compared to DayCent simulations with the default
- 600 CUE value for the structural pool (these had a negative model efficiency at all four sites; Fig. [A6\)](#page-47-0). While Aludeka experienced improved model efficiency for simulated changes in SOC stocks with the leave-one-site-out cross-validation , simulated the change in SOC much more accurately than with the default parameter set (EF of (from -4.17 to -1.84), the model efficiencies for Embu and Sidada slightly worsened (from 0.54 vs -1.3; LC of 88% vs 42%; Fig. [6\)](#page-25-0). The 95% credibility intervals of the simulated values contained 47% of the measured data. It to 0.33 in Embu and from 0.47 to 0.39 in Sidada). Even across sites,
- 605 the model efficiency (computed without Machanga) slightly decreased from 0.36 to 0.34 following calibration. As expected, <u>Machanga, for which the SOC stock data had been removed from the calibration dataset due to soil erosion at this site, exhibited</u> poor model efficiency (-3.6 after calibration).

Despite the reduction in model performance, the Bayesian calibration effectively captured the uncertainty in SOC stock changes in Aludeka, Embu and Sidada. Overall, 84% of measurements fell within the posterior credibility intervals, though

- 610 the evaluation was done with the site that was not used in calibration. While SOC changes were well captured in the control treatments across all sites, it should be noted that under- or overestimation of the change in SOC stocks from the start to the last year of the experiment was rather related to site than to treatment . In Embuwas most prominent in the treatment receiving 4 tC ha⁻¹ yr⁻¹ and this discrepancy varied by site. In Sidada, for example, all treatments except the control +N treatment that received 4 t C ha⁻¹ yr⁻¹ tended to have lower observed than simulated simulated than observed SOC losses, while in Aludeka
- 615 most treatments except the control -N treatment showed weaker predicted than observed SOC losses that received 4 t C ha⁻¹ yr⁻¹ showed a stronger simulated SOC gain than what was observed (Fig. [A7\)](#page-48-0). These tendencies are The large credibility intervals of the Bayesian calibration were also evident when comparing the temporal dynamics of measured versus with simulated SOC stocks (Fig. [7\)](#page-26-0). Most of the treatments were The difference between the 4 t C ha⁻¹ yr⁻¹ input and the control treatments were generally well simulated, but it is noteworthy that there is the considerable variability in the measured SOC stocks between 620 different time points likely contributed to the large posterior intervals.
	- 3.5 Simulated N₂O emissions and global warming potentialGHG balance

The simulations and measurements of N₂O emissions on a daily basis were not well aligned. This is clear from the negative modeling negative model efficiencies and the absence of a clear correlation between observed and measured values simulated N_2 O values indicated that model performance for daily N_2 O emissions was poor (Fig. [8\)](#page-27-0). Peaks While treatments with higher N

Figure 6. Simulated compared to measured changes in SOC stocks since the start of the experiment at the four study sites for the default initial DayCent parameter set (lefttop) versus the calibrated parameter set by leave-one-site-out cross-validation (rightbottom). The 724 data points correspond to the observations from the experimental treatments over 32 to 38 seasons, depending on the site. Symbols represent the different organic resource and chemical nitrogen fertilizer treatments. Grey bands show the 95% confidence intervals of measured (horizontal) values and the 95% credibility intervals of posterior distribution (vertical). Abbreviations: EF, Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation. <u>Across all sites model statistics without Machanga</u> (from which SOC data was excluded in the calibration process due to strong erosion): EF, 0.364; RSME, 5.199 t ha⁻¹; SB, 1%; NU, 22%; LC, 77% before and EF, 0.339; RSME, 5.11 t C ha⁻¹; SB, 9%; NU, 29%; LC, 62% after calibration, with 84% of measurements being in the 95% credibility interval of the posterior.

Figure 7. Measured (dots) versus simulated SOC stocks over time at the four study sites for the different organic resource and chemical nitrogen fertilizer treatments. Error bars represent 95% confidence intervals for measured data, the black solid line the simulation by the best parameter set for each site. Grey bands represent the 95% credibility intervals of the model posterior simulations, calibrated by leave-onesite-out cross-validation. Note that due to intense soil erosion, data from Machanga was not used in the calibration process.

Figure 8. Simulated compared to measured N₂O emissions at the four study sites for the different organic resource and chemical nitrogen fertilizer treatments, based on the calibrated parameter set using leave-one-site-out cross-validation. Displayed are the measured versus modelled per treatment for the days where measurements were conducted (top) and for the mean of cumulative flux measurements per season using the trapeziod method (bottom). The 808 data points (top) correspond to the daily measurements from the experimental treatments over one to two seasons, depending on the site. Symbols represent the different organic resource and chemical nitrogen fertilizer treatments. Error bars represent 95% confidence intervals based on BC (simulationsmeasurements) and variance credibility intervals (measurementssimulations). Abbreviations: EF, Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation.

- 625 loads had both higher simulated and measured N_2O fluxes compared to those with lower loads, the peaks of N_2O emissions were often simulated on different dates than the measurements, but treatments with higher N loads tended to have higher simulated and higher measured N₂O fluxes. This was most noticeable in +N compared to -N treatments (Fig. [A8\)](#page-50-0). For Conversely, for cumulative N₂O emissions per seasonon the other hand, there was a much better alignment better agreement between the simulated and measured values. All sitesshowed positive modeling efficiency (highest EF 0.34 for Aludeka, lowest EF 0.21
- 630 for Machanga, except Machanga, showed positive model efficiencies (highest in Embu, 0.62; lowest in Sidada, 0.03; Fig. [8\)](#page-27-0). Additionally, the correlation between cumulative simulated and measured N₂O emissions was much higher notably higher for the cumulative emission fluxes than for daily emission fluxes (R^2 between 0.26 for Sidada and 0.81 for Aludeka 0.72 for Aludeka and 0.30 for Sidada, compared to \mathbb{R}^2 close to 0). for daily fluxes). Furthermore, despite some bias in Aludeka and Sidada, most of the error in seasonal N₂O emissions was not systematic (i.e., LC of 63 - 95%).
- 635 The simulated changes in SOC and simulated cumulative seasonal N₂O emissions , showed positive global warming potentials (GWP) revealed a positive GHG balance for all treatments at all sites (Fig. ??). No treatment acted as a greenhouse gas sink, but the amount Q). Yet, the magnitude of emissions, as well as the contribution relative contributions of N₂O and CO₂, differed strongly between sites and treatments. In For instance, in the control -N treatment, it ranged from 1.4 emissions ranged from $2t$ CO₂ equivalent ha⁻¹ yr⁻¹ in Aludeka to 5.1 at Aludeka to 6 t CO₂ equivalent ha⁻¹ yr⁻¹ in Sidada and at Embu. The relative
- 640 contribution of N₂O from site to site also differed strongly by site. In At Aludeka, for example, between 32 (CT+N) and 82% $(FYMA+N)$ of the simulated GWP in the +N treatments all positive GHG balance values in the 4 t C ha⁻¹ yr⁻¹ treatments receiving farmyard manure, *Tithonia*, and *Calliandra* came from N₂O, while at all other sites, none of the treatments had more than 25% of GWP SOC acted as a sink of GHG. In contrast, at Sidada and Embu, most treatments had around one-third of GHG balance associated with N₂O emissions, with the remainder attributed to SOC losses. Compared to the control -N treatment,
- 645 which is closest to the low-input agriculture practiced by most smallholder farmers, all organic resource input treatments in the -N treatments were projected simulated to have lower emissions (Fig. ??). The reductions ranged from -0.2 t Q). Yet, including the $+N$ treatments, the changes ranged from an increase of CO₂ equivalent ha⁻¹ yr⁻¹ to $+a$ reduction of 2.5 t CO₂ equivalent ha⁻¹ yr⁻¹. Apart from that, the only Embu was the site where the addition of mineral N (+N treatment) could lead to a higher simulated GWP per ha than led to the strongest increase in simulated GHG balance compared to the control -N treatmentwas 650 Embu, and this was only the case for the treatments of *Calliandra, Tithonia* and farmyard manure in both 1.2 and 4 t of C input
	- ha⁻¹ yr⁻¹. Furthermore, Embu and Machanga tended to have high $_{\odot}$

Finally, there were site- and treatment-specific differences in the yield-scaled GHG balance. The control, maize stover and sawdust treatments -N had the highest simulated emissions per kg of maize yields (0.9 to 1.6 and 0.8 to 2.5 grain yield across sites $(1 \text{ to } 1.5 \text{ kg CO}_2$ equivalent per kg of yield, respectively, due to lower yield). On the contrary, the simulated emissions 655 ranged between 0.1 and 0.7 kg $CO₂$ equivalent per kg of yield in Aludeka and between 0.4 and 0.9 kg $CO₂$ equivalent per kg of yield in Sidada. Notably, none of a lack contrast, the farmyard manure, *Callianda* and *Tithonia* treatments at inputs of 1.2 to

 Cat^1 , Tr^1 in the +N treatments in Sidada and Aludeka had higher emissions than treatment and at 4 t Cat^1 , Tr^1 in both -N and $+$ N treatments tended to have the lowest simulated emissions at all sites (around 0.5, 1 and 0.6 kg CO₂ equivalent per kg of yield at Aludeka, Embu, and Sidada, respectively).

Figure 9. Cumulative simulated global warming potential greenhouse gas (GHG) balance of N₂O emissions and CO₂ emissions due to loss of SOC at the four study sites for different organic resource and chemical nitrogen fertilizer treatments, combined throughout the simulated period (16 years for Aludeka/Sidada; 19 years for Embu/Machanga). The global warming potential GHG balance is expressed in CO₂ equivalent over a 100-year horizon.

4.1 Robustness of the Bayesian calibration shown by **eross evaluation** eross-validation

As shown by our the leave-one-site-out cross-validation (Figs. [3](#page-20-0) and $\frac{224}{12}$), the Bayesian calibration considerably improved the predictive capability of DayCent to predict for maize grain yield , aboveground biomass and changes in SOC stocks at the four long-term ISFM experimental and aboveground biomass across sites. The model evaluation statistics from this calibration 665 exercise were comparable to those of other reported in recent publications that also combined the predictions of crop yield and SOC [\(Necpalova et al., 2018;](#page-55-3) [Levavasseur et al., 2021;](#page-54-9) [Nyawira et al., 2021\)](#page-55-2). However, while these studies generally showed a better simulation of crop yield than SOC, which is in contrast to our results, where crop yield and SOC were simulated equally well. Of the three types of measurements, simulated changes in SOC stocks related to different treatments were most improved after model calibration, reducing the strong bias towards simulated gains in SOC, where instead losses were measured. In 670 general, our study diverged. We found that while better yield simulations compared to SOC simulations were evident at the Aludeka and Machanga sites with soils of low clay content, the results were different at the Embu and Sidada sites with clay-rich soils. Here, SOC stock changes were more accurately simulated than maize grain yield. This, together with the fact that improved simulation of maize grain yield and aboveground biomass was coincided by a lower model performance in simulating SOC changes (Figs. [6\)](#page-25-0), suggests that no single best parameter set exists for the current version of DayCent 675 to accurately represent the conditions at all four sites. In that regard, the sereening of the model parameters with the global sensitivity analysis proved valuable in reducing the complexity of the calibration problem. The most sensitive parameters (Table [1\)](#page-13-0)were well constrained, while the least sensitive parameters (aneref(3), ppdf(2) and ps1co2) were difficult to constrain. This suggests that a reasonable threshold for including a parameter in model calibration may even be greater than a total Sobol sensitivity index of 2.5%. This result is similar to discrepancy between the sites with clay-rich and clay-poor soils could indicate 680 that DayCent insufficiently includes soil textures effects on nutrient availability and SOC formation. Yet, drawing definitive

- conclusions from just four sites is probably not warranted. In the absence of data from more sites, it is preferable to apply the full range of possible parameter sets that are supported by the study of [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2), where the parameters with a total sensitivity index <10% were also poorly constrained. In our study, it was possible to constrain the most sensitive parameters (prdx(1), himax, dec(5)); exceptions were the two parameters pmco2(1&2) and clteff(1,2&4), but their correlation ($r = -0.43$)
- 685 is a reasonable explanation of why they could not be well constrained despite high sensitivity. Possibly, the algorithm cannot distinguish whether organic resources are poorly stabilized due to tillage disturbance, a fast turnover rate of the slow SOM pool, or a low carbon use efficiency of metabolic and /or structural litter pools. Such a correlation between SOM stabilization and turnover parameters is common in soil models (e.g. [Ahrens et al., 2014;](#page-51-7) [Laub et al., 2021\)](#page-53-10), especially if the SOM pools do not represent measurable fractions [\(Laub et al., 2020\)](#page-53-7). available data [\(Mathers et al., 2023\)](#page-54-10), rather than using only the single 690 best parameter set.

Robust predictions of crop yields and changes in SOC stocks, as achieved by our cross-validation, are an important basis for potential future upscaling exercises of crop yield and SOC model predictions to national scales. While many model calibration exercises often display an overly optimistic picture of the capacity of models to represent SOC dynamics, by displaying how well the models represent absolute levels of SOC (e.g., in [Nyawira et al., 2021;](#page-55-2) [Ma et al., 2022;](#page-54-11) [Levavasseur et al., 2021\)](#page-54-9), the

695 changes in SOC since the start of an experiment, shown in this study, are much more robust evaluation. Since models are typically parameterized to fit the observed SOC stock at the start of the experiment, absolute SOC will always closely resemble measurements, with the possible exception of experiments that run for many decades. The fallacy of this approach was shown by [Necpalova et al.](#page-55-3) [\(2018\)](#page-55-3); [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2), where the absolute SOC overoptimistically masks the bias of change in SOC stocks. This is also the case for the present study, as is clear from the results of the model simulations for the absolute SOC 700 stocks compared to the changes in the SOC stocks (Fig. ??). Since

Because our calibration shows a good fit and is free from serious bias even for model fit with observed mean yields and changes in SOC stocks (that is, 88% of the errors are LCand not systematic; EF is 0.55 across sites, with no overall major bias (positive EF and errors mostly consisting of LC), the ealibrated DayCent model can be used in a robust manner to estimate the change of SOC stocks under different ISFM management in Kenya. Furthermore, because the model evaluation and calibration

- 705 parameter set, especially the full posterior, appears suitable for upscaling of model simulations. However, on should keep in <u>mind that the season-to-season yield variability is captured less accurately than the mean yields (lower RMSE) and that changes</u> in SOC are better represented at sites with clay-rich soils than those with clay-poor soils. Because the model calibration and evaluation were performed at different sites , it seems reasonable to use DayCentfor other sites with diverse characteristics, it is reasonable to assume that DayCent, when applied to sites with similar climate and soil conditions, even beyond Kenyawill
- 710 provide satisfactory results with similar model uncertainties and errors. In that respect, while the leave-one-site-out crossvalidation is using the data most efficiently: for evaluation, we leave one site out, but for made efficient use of data for model evaluation, further model upscaling exercises, ideally should apply the full posterior model parameter set including all sites (Fig. [2\)](#page-19-0) should be used. A computationally less expensive alternative is to In that case, a computationally inexpensive exercise would use only the single parameter set with the highest likelihood best parameter set (Table [1\)](#page-13-0), while the full posterior
- 715 parameter set should be used to get estimates of the posterior credibility intervals for changes in SOC stocks.

4.2 Bayesian calibration suggests that SOC is lost at higher rates in tropical than in temperate soilsshows uncertainty of model parameters

To estimate the potential yield and long-term sustainability of cropping systems without major bias using biogeochemi-cal models, regionalized region-specific model calibrations are needed [\(Rattalino Edreira et al., 2021;](#page-55-9) [Yang et al., 2021\)](#page-57-5).

- 720 Therefore, while previous studies have simulated crop productivity under ISFM and similar practices with default parameter sets the default parameter values (e.g. [Nezomba et al., 2018;](#page-55-10) [Nyawira et al., 2021\)](#page-55-2), the results of our study indicate that especially to estimate the effect on SOC, local calibration is very much needed (Fig. [6\)](#page-25-0). underscore the importance of a local calibration, especially when simulations are done with a single parameter set. On the other hand, the similar ranges of the prior and posterior model parameter sets indicate that including prior knowledge into model parameters substantially improves
- 725 model performance compared to using default parameter values (e.g., see the poor model performance without including prior knowledge on ps1co(1&2)&rsplig; Fig. [A6\)](#page-47-0). In fact, the turnover values of the turnover rates of the slow and passive SOM pools was approximately two and eight times higher than in for our study sites were in alignment with those derived in a

recent Bayesian calibration of DayCent for temperate systems conditions [\(Gurung et al., 2020\)](#page-52-2), indicating a that the DayCent temperature function is well suited to handle the faster SOM turnover under tropical conditions, as expected. However, since

- 730 the SOM pools in DayCent do not correspond to measurable fractions and we did not have additional data (e.g., 14 C). constraining the related parameters is expected to be subject to high uncertainty (e.g. [Ahrens et al., 2014\)](#page-51-7). Nevertheless, our results of high SOM turnover in Kenya are in line with the results of two recent studies, which also found that the default parameterizations of the DayCent [\(Nyawira et al., 2021\)](#page-55-2) and the LPJGUESS model [\(Ma et al., 2022\)](#page-54-11) underestimated the loss of SOC in two other long-term experiments in Kenya. In our study, it is important to note that our sites were under natural
- 735 vegetation (i.e. forest) or fallow until relatively shortly before the establishment of the low Sobol total sensitivity indices of the maize productivity parameters for the SOC stocks suggest a limited importance of root input in the soil system for the storage of SOC. These results align with a statistical analysis of SOC stocks across depth at the same experimental sites [\(Laub et al., 2022a\)](#page-53-1), which found limited differences between cropped and bare plots, and with another recent tropical long-term experiment [\(Cardinael et al., 2022\)](#page-51-8), which estimated that less than 1 t of carbon input ha⁻¹ per year came from maize 740 roots.

Overall, experiments [\(Laub et al., 2023a\)](#page-54-4). Consequently, upon the start of cultivation, erosion and potentially accelerated decomposition (due to soil disturbance) occurred, and SOC has likely not yet reached a new equilibrium with C inputs from maize cultivation. Therefore, C loss is the dominant process occurring at the sites. The good simulations of these strong SOC changes using MAOC initialized SOM pools, a method not commonly used with DayCent, further supports suggestions to

- 745 move away from purely conceptual SOM pools [\(Abramoff et al., 2018;](#page-51-9) [Laub et al., 2024\)](#page-54-12). Such conceptual pools require many assumptions about the initial vegetation and soil conditions (e.g., in the considerably higher simulated SOM turnover rates in this study compared to those in temperate regions [\(Gurung et al., 2020\)](#page-52-2) suggest that the lower SOM stabilization potential of highly weathered minerals in tropical soils [\(Doetterl et al., 2015\)](#page-52-9) is not adequately accounted for in DayCent. DayCent only includes an effect of clay content. Possibly, the effect of weathered minerals is large for both slow and passive SOM
- 750 pools(increased turnover by 2^1 the spin-up modelling or estimation of SOM pool distribution). In fact, the high uncertainty about initial vegetation, and 2^3 in this study, respectively) and is not adequately represented by texture alone. It was recently shown that the Millenial model, which has measurable pools , could better simulate the global SOC distribution than the CENTURY model, which has conceptual pools [\(Abramoff et al., 2022\)](#page-51-10).Recent attempts to move DayCent in that direction have also shown some promising results (e.g. [Dangal et al., 2022\)](#page-52-10). Furthermore, it is possible that hand tillage twice a year and
- 755 potential erosion also played a role in the high SOC losses that informed these fast turnover rates. Because DayCent does not include erosion and erosion was not measured in the experiments, the exact role of these processes is hard to determine. Therefore, the different calibrations of the DayCent model in our study and in [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2), suggest that the calibration developed in this study should only be used for soils of similar mineralogy and under a similar climate and for a similar maize cropping system.
- 760 4.3 Maize crop module is more universally applicable than soil carbon module

Although the mean yields per treatment were well represented and the provisioning of N via organic resource mineralization was well captured, as demonstrated by a good agreement between the mean simulated and measured yields in the -N treatments (Fig. [5\)](#page-23-0), the improvement in the simulated maize grain yield through the joint Bayesian model calibration of SOM pools and the maize crop highlights the interconnectedness of bothtime and management since site conversion, was a major reason

- 765 to move away from the model spin-up and site history run usually typically done with DayCent. Thus, even if the crop parameterization is correct, as indicated by the low difference between initial and calibrated maize parameters, too low SOM pool turnover rates, by underestimating mineralization of N from soil, results in too high demand of maize for mineral N addition to produce a suitable yield. This can be seen in the poor simulation of the low input treatments of Sidada before calibration and their improvement after calibration (Fig ??). Interestingly, in contrast to SOC turnover rates, the values of the
- 770 maize crop parameters in this study were close to the set of default parameter values of DayCent, especially the maximum production capacity (prdx(1)). This our study provides additional support to modify DayCent, incorporating measurable SOM pools (e.g. [Dangal et al., 2022\)](#page-52-10).

<u>In that sense, the similarity of our DayCent model calibration with that of [Gurung et al.](#page-52-2) [\(2020\)](#page-52-2) and earlier studies, despite</u> using different model initialization approaches, indicates the broad applicability of DayCent. It suggests that the traits of the

- 775 maize are universally represented in DayCent , whereas the turnover of the SOM is not. In this context, the changes in the values for SOM turnover and maize traits in DayCent are representative for temperate to tropical conditions. The adjustments made to the values of optimal and maximum temperature for maize growth (ppdf(1) and ppdf(2)) could be attributed to the adaptation of local maize species local maize varieties that are adapted to the higher temperatures in Kenya. For example, [Yang et al.](#page-57-5) [\(2021\)](#page-57-5) conducted a region-specific Bayesian model calibration of the DayCent maize growing parameters and found ppdf(1)
- 780 to very yary between 26 and 32 °C. Therefore, the different optimal temperatures (33°C) and highest temperatures (40°C) for the calibration of maize to US conditions by [Necpálová et al.](#page-55-1) [\(2015\)](#page-55-1) do not contradict the range of parameters of our study. However, the differences in model performance by site shows that the broad representativeness of DayCent comes at the cost of model simplification and site-specific model performance. A main reason for this may be that DayCent model formalisms do not include the latest mechanistic understandings of the role of microbes in SOM decomposition [\(Laub et al., 2024\)](#page-54-12), and
- 785 the sorption kinetics of carbon to minerals for SOM protection [\(Abramoff et al., 2018;](#page-51-9) [Ahrens et al., 2020\)](#page-51-11). Additionally, Daycent does not fully consider that a lot of stabilized SOC is formed by microbes from metabolic and not structural litter [\(Cotrufo et al., 2013;](#page-52-6) [Kallenbach et al., 2016\)](#page-53-6). For example, it was recently demonstrated that the Millenial model, which includes measurable SOM pools and improved kinetics of carbon sorption better predicts SOC stocks at the global scale than the CENTURY model, which has conceptual SOM pools [\(Abramoff et al., 2022\)](#page-51-10). While model calibration can compensate for
- 790 deficiencies in mechanistic accuracy at a single site [\(Laub et al., 2024\)](#page-54-12), this is likely not possible across sites with different conditions.

An interesting observation is that while the model bias for the mean yield of maize appears to be maize yield was treatment specific (i.e., the mean yields of $+N$ treatments of farmyard manure at 4 t C ha⁻¹ yr⁻¹ at all sites and of *Tithonia* at the same rate in all but Sidada, were underpredicted by DayCent), while the bias for SOC stocks was mostly site specific (i.e., SOC loss in

795 Aludeka was underpredicted, while overpredictedin Embu). As discussed above, the site bias of SOC is likely due to formation

in Aludeka at 4 t C ha⁻¹ yr⁻¹ was overpredicted). A potential explanation for this site-specific bias for SOC is the fact that soil DayCent was developed under the paradigm of SOM formation occurring mainly from recalcitrant humic compounds in the soil. Alternatively, it might indicate that soil texture alone is insufficient to explain the mineralogy-driven storage potential of SOC (e.g. [Reichenbach et al., 2021;](#page-56-9) [Mainka et al., 2022\)](#page-54-13). On the other hand, our <u>Finally, our model</u> sensitivity test to mineral N 800 input inputs suggests that the maize yield bias at high N is due to DayCent's inability to capture yield increases above 100-150

kg N per ha and season <u>at the four sites</u> (Fig. [A5\)](#page-45-0); the +N treatments of *Tithonia*, *Calliandra* and farmyard manure at 4 t C ha⁻¹ yr⁻¹ supplied on average >250 kg N per ha and season. Another reason may be Here, it should be noted that DayCent does not include other potential beneficial effects of <u>organic resource</u> treatments, such as increased pH from farmyard manure application [\(Xiao et al., 2021;](#page-57-6) [Mtangadura et al., 2017\)](#page-55-11)and higher nutrient retention and ₂ or improved water infiltration of 805 treatments that maintained maintain SOC stocks compared to those that showed a decline of SOC reduce them.

4.3 N₂O emissions and global warming potentialGHG <u>balance</u>

In general, the poor match between *daily* observed and measured *daily* N₂O emissions (Fig. [A8\)](#page-50-0) illustrates the difficulty of simulating the timing of microbial processes, $\frac{\text{in-throught}}{\text{turb}}$ which nitrate (NO₃⁻) is converted to N₂ and N₂O gasses, with intermediate complexity models models of intermediate complexity such as DayCent. Several recent studies show that poor 810 simulation of N₂O emissions by process models is common [\(Zhang and Yu, 2021;](#page-57-7) [Wang et al., 2020\)](#page-57-8), which is attributed,

- among other factors, to a Qne reason is the poor representation of soil hydraulics. For example, [Sommer et al.](#page-56-10) [\(2016\)](#page-56-10) found mainly overestimated N₂O emissions in Kenya. [Gaillard et al.](#page-52-11) [\(2018\)](#page-52-11) reported that there is a bias in simulated N₂O emissions by most models, postulating an underestimation of strong N₂O flushes. This also seems to be the case in our study, at least for treatments with high N inputs such as farmyard manure +N. Without resorting to more intricate water flow equations, it could
- 815 be difficult to make further improvements to the simulation of soil water content and N₂O emissions, particularly in terms of accurately predicting daily and hourly events. DayCent is driven by inputs that are only resolved at daily time steps and fed with pedotransfer functions that are poorly represented in the tropics [\(Van Looy et al., 2017\)](#page-56-11). moisture dynamics by the 'tipping bucket' soil water balance approach and that soil gas diffusivity is not explicitly simulated [\(Zhang and Yu, 2021;](#page-57-7) [Wang et al., 2020\)](#page-57-8)

. However, the fact that cumulative N_2O emissions were better eaptured simulated than daily emissionsand that , there was no 820 systematic under- or over-prediction of cumulative N_2O emissions, does suggest that and simulated N_2O emissions were generally reasonably well predicted with this current DayCent calibration. This is important for the predictions of the GWP. Because the simulation of SOC change showedlow bias, we can conclude that this part of the GWP is well represented. Depending on the site and treatment, within the uncertainty range of measured N₂O emissions, demonstrates the suitability of

DayCent to represent average N₂O emissions with the current calibration. Given the limited bias in simulating SOC changes

825 and cumulative N₂O emissions showed, the DayCent simulations provide a reasonable first estimate of the GHG balance. Nevertheless, the contributions of N₂O emissions contributed between 80% (to the GHG balance of up to 100% (at Aludeka) and up to 20% of the GWP (between 10 to 50% (at the other sites; Fig. ??). However, the Q), are subject to high uncertainty, as evident from the measurements. The larger confidence intervals of the measured compared to the simulated cumulative N₂O emissions suggest that the DayCent model cannot fully represent the variability. Although Thus, although DayCent's

830 simulation simulations of N₂O emissions is are superior to using emission factors factor approaches [\(dos Reis Martins et al.,](#page-52-12) [2022\)](#page-52-12), simulating N₂O emissions remains challenging and highly uncertain due to the complexity of the processes involved and the high temporal and spatial variability of N_2Q emissions.

Despite this uncertainty, which has not yet been resolved, our analysis of yield-scaled and area-based GWP showed the $\frac{1}{2}$ importance of the unit of reference. Our unresolved uncertainty, our modeling results show that ISFM with maize monocropping

- 835 cannot be seen as a negative emission technology. All treatments had a positive absolute GWP, which is consistent with the reported losses of SOC in long-term maize cultivation in SSA [\(Sommer et al., 2018;](#page-56-12) [Laub et al., 2022a\)](#page-53-1). It is also consistent with all ISFM options in a maize monocropping system have a net positive GHG balance, aligning with the prevalent trend of SOC losses in recently established (< 50 years) maize systems in SSA [\(Sommer et al., 2018;](#page-56-12) [Laub et al., 2023a\)](#page-54-4). The findings also support the postulate that closing SSA yield gaps will boost absolute yield gaps in SSA will increase N₂O emissions [\(Leit-](#page-54-5)
- 840 [ner et al., 2020\)](#page-54-5). However, the strong-large differences in the yield-scaled GWP GHG balance between treatments, such as a 72, 32, 63 and 14 the 30 to 60% lower yield-scaled GWP GHG balance in the FYM 1.2+N treatment compared to the control-N treatment across the sites, indicate that ISFM has the potential to produce crops with relatively lower GHG emissions than noor low-input input systems. Specifically, the ISFM treatments with low-emissions and high yields, show that the yield-scaled \hbox{GWP} is highly relevant in practical terms. Low-emission and high-yield ISFM treatments , such as FYM 1.2+N, producing that
- 845 $\frac{1}{\text{prod}}$ between 2 and 4 t of yield per season at emissions of between 0.2 and 1 kg CO₂ equivalent per kg of yield, are a suitable mitigation practice compared to standard practice, control the control treatment with little or no inputs of organic and/or chemical fertilizer. The difference in the yield-scaled GWP ranges of +N treatments that existed between western Kenyan sites (Aludeka and Sidada; 0.1 to 0.5 kg $CO₂$ equivalent per kg of yield) compared to central Kenyan sites (Embu and Machanga; 0.8 to 1.1 kg $CO₂$ equivalent per kg of yield), furthermore, show that N fertilizer should only be applied to responsive soils
- 850 [\(Sileshi et al., 2022\)](#page-56-13) to avoid high N₂O emissions at minimal yield. Consequently, sustainable intensification and mitigation of greenhouse gases can go hand in hand.

4.4 DayCent is suitable to upscale simulations of "real" ISFM, but not sensitive for very limit<u>ed sensitivity to</u> high N inputs

Because mean yields were represented well maize yields across sites were reasonably well represented by the calibrated version 855 of DayCent, it can be used to upscale to national levels and for upscaling to predict the potential of ISFM to lower yield gaps impact of ISFM in lowering yield gaps at national levels. However, the levelling off-plateauing of mean yields at very-high N loads (Fig. [A5\)](#page-45-0) indicates that it DayCent may not be suitable to estimate the for estimating maximum achievable yields (e.g., [Ittersum et al., 2016\)](#page-53-11)and it should , and should thus be restricted to <u>yield</u> predictions for medium input levels of NN input levels. Given that the historical rates of N fertilizer application in Kenya were are less than 50 kg of N ha⁻¹ [\(World-Bank, 2021a\)](#page-57-9), the

860 model seems suitable to simulate the effect of applying real ISFM, which aims at implementing realistic' ISFM practices, which target maximum N use efficiency [\(Vanlauwe et al., 2010\)](#page-56-0), with N $\frac{input}{input}$ rates considerably below the maximum N rates of the simulated field trials used in the field experiments of this study (e.g., 80 kg N per season; [Mutuku et al., 2020\)](#page-55-12). The prediction of mean yields worked well maize yields was reasonably good for *Calliandra* and farmyard manure treatments at 1.2

and 4 t C ha⁻¹ in the -N treatmentand was also acceptable λ as well as for CT+N, i.e., all treatments that supply N at the desired 865 rate for ISFM. Hence, at these N-levels, simulated mean maize yields are likely representative of the ISFM yield potential. The poorer performance of sawdust is less relevant for upscaling, because this is a treatment for scientific understanding (testing if SOC really forms more efficient from lignin rich materials; [Palm et al., 2001b\)](#page-55-13). <u>achievable yield through ISFM.</u> In summary, the mean yield potential and the change in the SOC stocks were well represented, so the model calibration seems

- suitable for assessing the long-term effect effects of relevant ISFM treatments practices on soil fertility, maize yield, and 870 greenhouse gas GHG emissions as well as their trade-offs. Since, given the good representation of mean yield potential and SOC changes by the model. Nevertheless, since year-to-year variations of yield yield variations were not captured very well, it is questionable how well the current calibration could represent well by DayCent, it remains uncertain how effectively the current model calibration can simulate scenarios of climate change, where temperature and precipitation patterns will become more erratic. In the absence of major pests (which in the trials experiments were controlled), the yearly variation in variations
- 875 in seasonal precipitation and temperature should be responsible for the are responsible for these differences, and if these are not well represented, we cannot trust that we can apply DayCent outside of the applicability of DayCent beyond the climatic range that it was calibrated for is questionable.

5 Conclusions

In this study, we demonstrated the effectiveness of jointly simultaneously calibrating the SOM and plant modules of DayCent

- 880 to simulate maize productivity and changes in SOC stocks under integrated soil fertility management (ISFM) in Kenya, using a Bayesian calibration . The calibration successfully constrained the most sensitive approach. Our study showed the importance of choosing correct values for model parameters, which were identified by a global sensitivity analysisand using the full posterior parameter set is the best solution to assess the uncertainty of model outputs. Although the default initial DayCent maize plant parameterization represented the tropical conditions in Kenya well acceptably (i.e., the highest probability posterior
- 885 parameter values were close to the default initial parameterization), the highest probability posterior SOM turnover rates were two and eight times faster than the default for the passive and slow SOM pool, respectively. This indicates that there is the potential for large losses of SOC in highly weathered tropical soils. However werall model performance for maize grain yield and aboveground biomass was improved after calibration using local data. However, better yield simulations partially came at the cost of poorer SOC simulations at some sites. Furthermore, SOM turnover was subject to high uncertainty , showing and
- 890 biased for clay-poor sites, indicating that the current module structure suboptimally inadequately captures SOM dynamics in highly weathered tropical soils. Nevertheless, our Qur leave-one-site out cross validation showed that the calibration-derived parameter set is robust for upscaling of the model the model simulations to larger areas in Kenya, particularly when applying the full posterior parameter set. At the same time, while mean maize grain yields were much better represented than well simulated, the year-to-year variability of yields, posing the question whether the yield variability raised concerns about the
- 895 and the model's ability to capture the short-term effects of climate change can be adequately captured by DayCentadequately. Finally,

while no ISFM treatment was predicted to act as an absolute a net sink of greenhouse gases, yield-scaled emissions were lowest in treatments with high and intermediate yields <u>exhibited the lowest yield-scaled emissions</u>.

Code availability. To get the latest version of DayCent, we suggest to contact the developers directly, who in our case kindly provided the latest DayCent version.

900 *[D](https://doi.org/10.25502/wdh5-6c13/d)ata availability.* The data sets used for the calibration of this study are available under the IITA data repository. For SOC: [https://doi.org/](https://doi.org/10.25502/wdh5-6c13/d) [10.25502/wdh5-6c13/d.](https://doi.org/10.25502/wdh5-6c13/d) For yields and biomass: [https://doi.org/10.25502/be9y-xh75/d.](https://doi.org/10.25502/be9y-xh75/d)

Author contributions. JS, MN and ML designed the modeling exercise. ML summarized the data, conducted the modeling exercise and prepared the original draft. MWMM, DM, RY, SMN and WW managed and maintained the long-term experiments. ML, SMN, MN, WW, MvdB, MC and JS were involved in the various sampling campaigns. MC, MN, BV and JS acquired funding for the long-term experiments. 905 All co-authors contributed in writing and editing of the final submitted article.

Competing interests. All authors declare that they have no conflict of interest.

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Appendix A: Appendix

920 A1 Site and organic resource characteristics

Table A1. Locations, soil properties and climatic conditions of the study sites. Soil properties are given for the 0 - 15 cm depth layer. Coordinates are given in the WGS 84 reference system. The table is adopted from [Laub et al.](#page-54-14) [\(2022b\)](#page-54-14) under the creative common license 4: http://creativecommons.org/licenses/by/4.0/

*Means calculated based on measured data from 2005 to 2020

Table A2. Mean measured chemical characteristics (and 95% confidence intervals) of organic resources applied at all sites. Measurements were available from Embu and Machanga from 2002 to 2004, all sites from 2005 to 2007 and in 2018. Significant differences in residue properties were found between the different organic resources, but not between sites and years. Same letters within the same row indicate the absence of significant differences for that property $(p < 0.05)$. Abbreviations: n.c. = not classified * according to [Palm et al.](#page-55-14) [\(2001a\)](#page-55-14). The table is adopted from [Laub et al.](#page-54-4) [\(2023a\)](#page-54-4) under the creative common license 4: [http://creativecommons.org/licenses/by/4.0/.](http://creativecommons.org/licenses/by/4.0/)

Table A3. DayCent model parameters (and feasible ranges) of parameters which were not included in the Bayesian model calibration due to a Sobol total sensitivity index $\leq 1\%$.

Figure A1. Prior compared to posterior parameter distribution resulting from increasing Map displaying the ranges location of the uncertainty based Bayesian calibration. Dashed vertical lines represent the default parameter sets. The posterior distributions are based on all four study sitescombined.

Correlation of parameters from the posterior parameter sets. The posterior distributions are based on all four sites combined.

A2 Subsoil SOC stocks for scaling SOC

A3 Barplots of SOC and comparing measured and simulated mean yield

Figure A2. Barplots of simulated and measured change of Subsoil SOC stocks until 2021 from cross-validation for the 2.5-4.7 kt ha⁻¹ equivalent soil mass layer, at corresponding to an approximate soil depth of 15-30 cm. Displayed are t<mark>he four study sites for least square</mark> means estimated by the different organic resource linear mixed model described in [\(Laub et al., 2023a\)](#page-54-4) for planted plots by treatment (left) and chemical nitrogen fertilizer treatmentssite (right). Error bars represent display the 95% confidence intervalsbased on BC. Same lowercase letters indicate the absence of a significant difference in SOC stocks between treatments at the same site (simulationsleft figure) and variance or between sites (measurementsright figure; all $p \le 0.05$). Abbreviations: CC, Calliandra; CT, control; FYM, farmyard manure; MS, maize stover; SD, sawdust; TD, Tithonia Diversifolia. 0, 1.2 and 4 correspond to C additions of 0, 1.2 and 4 t C ha⁻¹ yr⁻¹

Figure A3. Correlation of parameters from the posterior parameter sets. The posterior distributions are based on all four sites combined.

Measured and simulated maize grain yields over timeAbbreviations: EF, at the four study Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation. Across all sites model statistics: EF, 0.755; RSME, 0.707 t ha⁻¹; SB, 12%; NU, 25%; LC, 63% for the different organic resource and chemical nitrogen fertilizer treatments yield; EF, 0.583;

RSME, 2.01 t ha⁻¹; SB, 5%; NU, 18%; LC, 77% for the uncalibrated (top) and calibrated DayCent model (bottom)AGB. Measured and simulated maize grain yields over timeAbbreviations: EF, at the four study Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation. Across all sites model statistics: EF, 0.755; RSME, 0.707 t ha⁻¹; SB, 12%; NU, 25%; LC, 63% for the different organic resource and chemical nitrogen fertilizer treatments-yield; EF, 0.583; RSME, 2.01 t ha⁻¹; SB, 5%; NU, 18%; LC, 77% for the uncalibrated (top) and calibrated DayCent model (bottom)AGB.

Figure A4. Mean simulated versus mean measured yield and aboveground biomass (AGB) from the leave-one-site-out cross-validation. Error bars represent the standard deviation of measured and simulated values over all years.

Measured and simulated maize grain yields over timeAbbreviations: EE, at the four study Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation. Across all sites model statistics: EF, 0.755; RSME, 0.707 t ha⁻¹; SB, 12%; NU, 25%; LC, 63% for the different organic resource and chemical nitrogen fertilizer treatments yield; EF, 0.583; RSME, 2.01 t ha⁻¹; SB, 5%; NU, 18%; LC, 77% for the uncalibrated (top) and calibrated DayCent model (bottom) AGB.

925 A3 Comparing measured and simulated mean yield

A4 Site specific sensitivities of yield to N fertilizer

Figure A5. N-Yield response curve by site of DayCent to varying levels of mineral N application (control + N treatment, without organic resources) using the calibrated DayCent parameters. This was done to explain why DayCent insensitive at high N levelsDisplayed are the simulated mean yields across all simulated seasons (32 in Sidada and Aludeka, 38 seasons in Embu and Machanga). The amount of mineral N was given applied per season in 50/50 the simulations was evenly split application, at between the two real actual application dates of mineral N in each season at each site.

A5 SOC stocks

Figure A6. Simulated compared to measured maize grain yields, abovoground biomass and change in SOC : 1st stocks at the four study sites for the default DayCent outputs initial parameter set before adjusting ps1co(left1&2)vs calibrated by leave-one-site-out cross-validation (right)&rsplig from 0.5 to 0.85. Grey bands denote show the 95% confidence intervals of measured (horizontal) values and the 95% credibility intervals of posterior simulated distribution (vertical)values. Abbreviations: EF, Nash-Sutcliffe modeling efficiency; RMSE, root mean squared error; SB, squared bias; NU, non-unity slope; LC, lack of correlation.

A5 Calibration improvement by SiteBarplots of SOC

Figure A7. Simulated compared to Barplots of simulated and measured changes in change of SOC stocks since experiment start for the default DayCent parameter set (top0-30 cm depth) vs the calibrated parameter set by leave-one-site-out until 2021 from crossvalidation(bottom). Grey bands denote₂, at the four study sites for the different organic resource and chemical nitrogen fertilizer treatments. Error bars represent 95% confidence intervals of measured based on BC (horizontal simulations) values and the 95% credibility intervals of posterior distribution variance (verticalmeasurements).

Simulated compared to measured yield for the default DayCent parameter set (top) vs the calibrated parameter set by

- 930 leave-one-site-out cross-validation (bottom). Grey bands denote the 95% confidence intervals of measured (horizontal) values and the 95% credibility intervals of posterior distribution (vertical).
	- $A6$ N₂O emissions

Figure A8. Temporal Example of the temporal development of measured (black) vs simulated (red) N₂O emissions by site. The black error bars represent the 95% confidence intervals due to spatial replication error, the red error bars represent the 95% credibility intervals of simulated N2O emissions resulting from parameter distribution of the posterior parameter set.

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