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The impacts of CENTURY model initialization scenarios on soil organic carbon dynamics simulation in French long-term experiments

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A R T I C L E I N F O

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A B S T R A C T

Process-based ecosystem models are used increasingly to evaluate the impacts of agricultural practices on soil organic carbon (SOC) stocks at various scales. One of the major sources of error and projection uncertainty in these models is the specification of the initial SOC pools sizes. However, few studies have examined errors and uncertainty over time and for various agricultural practices. The main purposes of our study were 1) to examine the impacts of initialization scenarios on CENTURY model V4.5 performance and 2) to quantify the initialization contribution to the total variance of error of the CENTURY model. We simulated the SOC dynamics of six well-characterized long-term experiments (LTEs) with 25 treatments across France, testing various agricultural practices (*i.e.*, inorganic and organic fertilization, various crop rotations and straw and residues removed) using the CENTURY model while keeping the standard parameters unchanged. We applied nine initialization scenarios, each characterized by a unique combination of crop management and relaxation procedures. These relaxation procedures consisted of shifting simulated SOC and nitrogen levels at the end of the initialization period until they matched the stocks at the beginning of the experiment. At the end of the initialization period, the distribution pattern of SOC pools was similar in all scenarios for all LTEs. The slow pool represented the largest proportion of total SOC stocks (average value of 61.5%), whereas the active and passive pools averaged 5.3% and 27.9%, respectively. The overall analysis of CENTURY performance indicated fair results for SOC stocks prediction (R^2 values of the nine initialization scenarios ranged between 0.50 and 0.75) but weak results for SOC change prediction (R^2 values of the nine initialization scenarios, ranged between 0.1 and 0.36). The root mean square error (RMSE) values were moderate compared to the total measured SOC stocks and their confidence intervals. The RMSE values ranged between 6.22 Mg ha^{-1} and 15.24 Mg ha^{-1}, which corresponded to 13.1% and 32.1% of the initial average total SOC stock for all LTEs, respectively. The highest values were recorded for the no relaxation procedures. CENTURY model errors (*i.e.*, simulated - observed SOC stocks) analysis showed a slight sensitivity to the initialization scenarios (approximately 6% of the total variance of the CENTURY error). However, the second-order interaction of scenarios and LTE contributed by 33.6%. Meanwhile, agricultural practices had the greatest impact on the variance of the CENTURY error (44.7%) compared to other factors. Our findings suggest that the contribution of the initialization to the uncertainty in projected SOC changes is negligible compared to the uncertainty related to the model itself and simulated systems characteristics.

1. Introduction

The Agriculture, forestry and other land use sector is responsible for nearly 25% of anthropogenic greenhouse gas (GHG) emissions, with approximately 9 to 12 Gt CO_2 eq yr^{-1} (IPCC, 2014). Based on FAOSTAT data and the IPCC Tier 1 approach using emissions factors, Tubiello et al. (2013) estimated that global agricultural non-CO_2 gases emissions increased by nearly 1% *per annum* between 1990 and 2010, with a slight increase in the growth rate after 2005, and contributed significantly to the total anthropogenic radiative forcing (IPCC, 2014). Therefore, keeping the global temperature rise below 2 °C by the mitigation of these agricultural GHG emissions is one of the most serious environmental challenges that the world is currently facing. Arable soils may act as a net sink of emitted CO_2 by sequestrating carbon and may

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thus help offset a substantial portion of GHG global mean forcing. This sequestration is possible through a range of optimal crop management strategies and could be substantial with widespread application (Lal et al., 2007; Zhang et al., 2014). These crop management strategies are receiving increasing attention from the scientific community (Smith et al., 2007; Luo et al., 2010a, 2010b) as well as countries that are developing research programs to achieve this objective. Among these research programs is the ambitious Future Earth research platform for global sustainability (www.futureearth.org) launched in 2015. Another promising research program is the "4 per 1000" initiative that stemmed from the 21st conference of the parties in Paris and aimed to offset atmospheric GHG emissions by the raising global soil organic carbon (SOC) amount by (4‰) annually (www.4p1000.org). Recently, the EU decision 529/2013 requires European Union's member states to assess ways to include those GHG fluxes resulting from agricultural practices into their national inventory reports (NIRs). However, accurate and reliable NIRs need to better consider both local conditions and agricultural practices by adopting the recommended IPCC Tier 3 methodology based on specific flux measurements and modelling (IPCC, 2014).

Process-based models simulating soil organic matter (SOM) dynamics are recognized as valuable tools for quantifying and understanding SOC dynamics in response to agricultural practices, particularly, in the context of rapid policy changes and/or to upscale experimental field results to the regional or national level (Paustian, 2000; Ogle et al., 2010). Most of these models, more than 250, represent SOC heterogeneity by conceptual pools (Manzoni and Porporato, 2007). Typically, these pools (3 to 5) have distinct specific mean residence times, are governed by first-order kinetics and are regulated by environmental conditions, which, in most cases, include temperature moisture and soil properties (Manzoni and Porporato, 2007). These pools are purely conceptual and are not defined by directly measurable properties (Zimmermann et al., 2007). In addition, the determination of their size remains challenging for accurate predictions of SOC stocks and their rate of change (Bruun and Jensen, 2002; Foereid et al., 2012). For instance, a passive or very slow SOC pool size could be a major source of uncertainty source since it is difficult to define and/or measure (Skjemstad et al., 1996; Trumbore, 2009). Falloon and Smith (2000) reported a large variation in the estimates of the age (*i.e.*, from hundreds to several thousand years) and size (*i.e.*, from 15% to 59% of the total SOC) of this pool between studies. Such differences in SOC pool size may lead to the parameters equifinality, also called identifiability, where multiple parameter combinations generate similar probability distributions for the observed variables, which leading to uncertainty in the projection of SOC dynamics (Tang and Zhuang, 2008; Luo et al., 2009; Sierra et al., 2015).

Many studies have questioned the optimal procedure for the initialization of the SOC pools sizes, but there is a lack of consensus regarding a common method (Bruun and Jensen, 2002; Wutzler and Reichstein, 2007; Carvalhais et al., 2008; Hashimoto et al., 2011). Three initialization methods are reported in the literature. The first initialization method consists of linking laboratory-measured fractions to functional model pools. The determination of SOC fractions sizes is performed by physical procedures, chemical procedures (Motavalli et al., 1994; Zimmermann et al., 2007; Wiesmeier et al., 2016) or a combination of the two (Trumbore et al., 1989; Leifeld and Kogel-Knabner, 2001). This initialization procedure is tedious for large-scale studies and has the inherent limitation that conceptual model SOC pools do not necessarily correspond to directly measurable fractions. In addition, fractionation procedures are not often described in detail, leading to reproducibility issues between laboratories, especially with different instruments or software platforms (Liao et al., 2006; Baker, 2016). Poeplau et al. (2013) set up a fractionation experiment to relate RothC model SOC pools to measured fractions and found significant differences among six laboratories, with the coefficients of variation ranging from 14 to 138%. The second initialization method consists of the use of pedotransfer functions (Wang et al., 2016). Weihermueller et al. (2013) developed a set of pedotransfer functions to obtain the initial values of *the* RothC model active carbon pool sizes using only the total organic carbon and clay contents. One limitation of this method lies in the specificity of these functions to a model and the studied soil, which requires adaptation when the method is used in other contexts. Nevertheless, Kwon and Grunwald (2015) constrained the initialization of CENTURY SOC conceptual pools with measurable Florida sandy soils properties. The authors found that clay content and hot-water soluble C, of these soils, were correlated to initial CENTURY active and slow SOC pools sizes inversely modeled from CO_2 evolved during laboratory incubation. The third method is the most commonly used procedure (Hashimoto et al., 2011). It consists of running the model iteratively (spin-up) with a repeated, constructed time series of climatic data and managed land use for hundreds or thousands of years to reach a prior assumption of steady state (equilibrium), where the ecosystem C inputs are equal to the outputs over a given time period (*e.g.*, Smith et al., 2005). However, aside from the computational demand and time-consuming aspect of this method, the system equilibrium state is unrealistic because of the legacy effect. This effect is caused by possible natural or anthropogenic disturbances and the long turnover rates of stable compounds (Wutzler and Reichstein, 2007, 2008). Nevertheless, if there is no information about the LTE historical land use or management available and/or there is no access to soil samples for SOC fractionation, *a* spin-up run remains the most appropriate initialization method. In our study, we used the widely applied process-based SOC model CENTURY to examine SOC dynamics in response to various agricultural managements in six French long-term experiments (LTEs). The aims of our study were to examine the impact of various initialization scenarios, based on spin-up runs, on CENTURY model performance and to statistically quantify their contribution to the model error. These initialization scenarios combine spinning-up over various historical management sequences, as well as the presence or absence of relaxation steps (*i.e.*, shifting the simulated SOC stocks to observed values at the beginning of the experiment).

2. Materials and methods

2.1. Study LTEs

We selected six well-characterized long-term experiments, with 25 treatments, from the AIAL data base and across France (Duparque et al., 2013; Bouthier et al., 2014). The LTE*s*/treatments selection was based on several criteria: i) at least three regular SOC stock measurements with repetitions, including the starting dates, to adequately follow the temporal evolution, ii) experiment duration exceeding 8 years, iii) information on lignin content of organic amendment was available, and iv) the experiment sets represent various agricultural practices (*i.e.*, inorganic and organic fertilization, rotation, straw and residues harvest) and pedoclimatic conditions. The main upper soil layer characteristics and management of the six LTEs, Saint Aoustrille, Auzeville, Boigneville, Feucherolles, Hessange and Tartas are described in Table 1. These experiments were carried out for various objectives, but we focused on SOC stocks dynamics.

The first LTE took place in, Saint Aoustrille, which is located in the Centre-Val de Loire region of France. The main purpose of this experiment was to evaluate the agronomic effect of leguminous, cereals and oleaginous cropping system combinations, and to examine the effect of previous crops on yields. Three crop rotations were established: Soybean - Winter Wheat - Rapeseed - *Sorghum*; Soybean - Sunflower - Pea - Rapeseed and Soybean - Winter Wheat - Rapeseed - Sunflower (Bouthier et al., 2014; Félix, 2015). The second *LTE* studied *was* Auzeville, *which* is located at the INRA experimental station *in* south *western* France near Toulouse (Colomb et al., 2007). The effect of inorganic phosphorus fertilization on yields was studied. Two doses of inorganic phosphorus fertilization, P0 (no P fertilization) and P4 (four-

Table 1
Main soil properties, climate and managements of study sites.

Location	Saint Aoustrille	Auzeville	Boigneville	Feucherolles	Hessange	Tartas
Coordinates	46° 93′ N 1° 93′ E	43° 52′ N 1° 43′ E	48° 19′ N 2° 22′ E	48° 53′ N 1° 58′ E	49° 20′ N 6° 30′ E	43° 52′ N 0° 44′ W
Mean annual temperature (C)	11.1	13.3	10.9	10.8	9.8	13.4
Mean annual P-PET (mm)	30.9	− 278,8	− 111,6	− 59,8	172	15.4
Experiment duration (yr)	9	41	40	15	7	21
Period of experimentation	1976–1985	1969–2010	1970–2011	1998–2013	1977–1985	1976–1997
Treatments	Crop rotation	Inorganic fertilization P	Residues management	Organic amendment	Crop rotation	Inorganic fertilization K
Treatment number	3	4	2	10	4	2
Main crop rotation	B/FB/R/S/P	W/M/S/SB/SG/FB/R	W/M	W/M	B/R/W/P	M
Soil depth (cm)	25	30	28	29	28	25
Bulk density (g cm^{-3})	1.2	1.4	1.46	1.32	1.3	1.4
Clay (g kg^{-1} soil)	351.4	256.5	255.1	150	344	61.5
Silt (g kg^{-1} soil)	502.2	323.3	667.6	783	512	133.5
Sand (g kg^{-1} soil)	146.4	393	77.2	67	144	805
pH	8.1	7.48	6.9	6.9	8	5.8
References	Félix et al., 2015	Colomb et al., 2007	Dimassi et al., 2014	Noirot-Cosson et al., 2016	Felix et al., 2015	Messiga et al., 2010

Bl: barley, Bt: beet, F: fababean, M: maize, P: Pea, Sb: soybean, Sf: sunflower, Sg: sorghum, R: rape seed and W: winter wheat.
P: precipitation (mm), PET: potential evapotranspiration (mm), Mean annual P-PET (mm) calculated for the whole study period.

fold mean annual P uptake of the crop), were applied. The Boigneville LTE, located in northern France, focused on the experiment referred to as "Experiment A" and tested the effect of residue management using two treatments: i) crop residues returned to soil and ii) crop residues removed for 12 years. The grain Maize - Winter Wheat crop rotation was established with only inorganic fertilization applied in accordance with recommended practices (Dimassi et al., 2014). The Feucherolles ongoing experiment, located in northern France, was set up in the frame of the INRA-Veolia collaboration project named QualiAgro. The aim of the experiment was to evaluate the environmental and agronomic impact of repeated applications of organic amendments. The field was cropped mainly with Winter Wheat and grain Maize. Four organic fertilizers were tested: dairy farmyard manure (FYM), municipal solid waste compost (MSW), bio-waste compost (BIO) obtained by composting green wastes and home-sorted municipal biowastes, and co-compost of green waste (70%) and sewage sludge (30%) (GWS) and a control treatment. These organic fertilizers were applied at a rate of 4000 kg C ha^{-1} every two years and crossed with two mineral N doses (Annabi et al., 2011; Peltre et al., 2012; Noirot-Cosson et al., 2016). The Hessange experiment was established at the experimental station of Arvalis-Institut du vegetal in the Moselle Department northeast France. The purpose of the experiment was to evaluate the agronomic and environmental performances of three cropping systems combining leguminous, cereals and oleaginous. Three crop rotations were established: Rapeseed - Winter Wheat - Soybean - Pea - Winter Wheat, Rapeseed - Winter Wheat - Rapeseed - Spring Pea and Rapeseed - Spring Pea - Fababean - Spring Pea (Bouthier et al., 2014). Lastly, the Tartas trial, located in south-western France, was carried out by the INRA. The objective of this study was to investigate the effect of mineral fertilization using two rates of potassium in the form of K_2O on continuous Maize cultivation yield with residues returned to the soil (Schneider, 2003).

2.2. CENTURY model description

The CENTURY model is widely used to simulate long-term SOM dynamics across a wide range of ecosystems, including grassland, cropland, savannah and forest, under various environments, management and for timescales ranging from years to centuries with a monthly time step (Parton et al., 1987, 1988). CENTURY has been successfully applied for long-term experiments and at different scales, ranging from national and regional to plot-level (Ogle et al., 2010). The model simulates nitrogen, phosphorus and sulphur dynamics as well as plant growth. The soil organic matter submodel is based on multiple compartments: surface and below ground structural and metabolic pools as well as active, slow and passive SOC pools (Parton et al., 1988). In the CENTURY model, plant residue is divided into structural C pools and metabolic C pools, according to the lignin to N ratio of the litter. The active C pool includes live microbes and microbial products with short turnover time periods (1–3 months). The slow C pool represents resistant plant materials originating from structural plant materials and physically protected soil microbial products, with turnover times of between 10 and 50 years. The passive C pool contains physically and chemically stabilized C, which is resistant to decomposition and has a turnover time between 400 and 4000 years. The turnover time of bulk SOC is considered a function of turnover time in specific C pools, soil moisture and soil temperature (Parton et al., 1987; Parton and Rasmussen, 1994). The major input variables are soil texture, weather data, crop sequence and management events (*e.g.*, tillage, fertilization, irrigation, harvest). Software and documentation are freely available on the web at https://www.nrel.colostate.edu/projects/century. In this study, we used a modified version 4.5 of CENTURY with the default parameters values kept unchanged.

2.3. Plant production calibration and setting of initialization scenarios

2.3.1. Plant production calibration

In this study, plant production was not simulated correctly (data not shown), most likely as a consequence of the crops and cultivars that belonged to our sequences not being well calibrated. Therefore, we kept the crops parameters unchanged and we calibrated the crops derived from C inputs using the observed yields. This was done in three steps. First, the biomass of aboveground crops residues returned to soil was estimated using the harvest index based on grain yield measurements (Beaudoin et al., 2008). Belowground biomass was calculated using methods described previously (Dubrulle et al., 2004). The C content of dry mass was assumed to be 42% and 38% in the aboveground and belowground residues, respectively (Justes et al., 2009). Second, we ran the model for all experiments and recorded, for each grown plant, the simulated plant-derived C inputs (Cin^{sim}) and compared them to the simulated plant-derived C inputs estimated from observed yields (Cin^{obs}) by calculating the ratio Cin^{sim}/Cin^{obs}. Third, under the assumption that the simulated plant-derived C inputs were proportional to the simulated plant production, we rescaled the simulated monthly plant production using this scaling factor for each crop cycle and reran again the simulations using this rescaling. This assumption was checked later afterward by ensuring, on a monthly basis that the simulated plant-derived C inputs were close to Cin^{obs}, during the calibrated simulations.

2.3.2. Setting of initialization scenarios

In this study, we chose to use the commonly used initialization method. This method consisted of running the model iteratively for thousands of years to initialize CENTURY SOC pool size. The objective was to be as close as possible to the initial SOC state at the start of trials. The monthly weather data inputs for the initialization period were taken from the weather database SAFRAN from 1960 to 2011 (Joly et al., 2010), covering the entire French territory on an 8 × 8 square km grid. We constructed time-series data of weather by drawing randomly climatic years from the period 1960–1989 within the SAFRAN database. The 1989 *year* was chosen, after which the French data records started changing because of climate change. Our scenarios did not include forest or grassland as land use. This choice was justified by recent studies that have highlighted extensive European deforestation since 1000 BCE (Kaplan et al., 2009). Furthermore, Lugato et al. (2014a) reported that the current cultivated area are fertile and has likely been under continuous cropping since at least 2000 years. We applied nine initialization scenarios consisting of three cropping systems (IS1, IS2 and IS3), hereafter referred to as managements, combined with three relaxation techniques. These relaxation techniques included the absence of relaxation (NR), fast relaxation (FR) and slow relaxation (SR) (Table 2).

Cropping systems used for initialization.

The first management (IS1) consisted of repeating the first five years of the current experiment rotation. The second management (IS2) was a typical 4-year rotation with a meadow, Wheat, Barley and fallow period called 'maggese' spanning the 0–1699 period, followed by a crop rotation without fallow until the beginning of the experiment. This management was adapted from Lugato et al. (2014b) who reported that this agricultural system was practiced by European farmers three millennia ago. The last crop management (IS3) was similar to IS2 until 1950, when the crop rotation was switched to the first five years of the experiment. All managements were conducted with low fertilization and moderate tillage. These scenarios were most likely close to experimental LTE's historical land use and management, and they generated different C input and, consequently, different SOC stocks and pools sizes at the end of the initialization. This difference between scenarios allowed us to examine the model behavior, when the modeled SOC stocks are far from the initial measured values. In addition, this initialization procedure helped determine the best scenario to initialize the CENTURY model for use at the regional or national levels when information on the historical management is not available, or when there is uncertainty regarding management.

Table 2
Initialization scenarios description.

	Management		Relaxation		
	Crop rotation	Period (year)	No relaxation (NR)	Fast relaxation (FR)	Slow relaxation (SR)
IS1	5 first years of the current experiment	1-Start of the experiment	IS1NR	IS1FR	IS1SR
IS2	M-WW-B-F M-WW-B	1–1699 1700-start of the experiment	IS2NR	IS2FR	IS2SR
IS3	M-WW-B-F M-WW-B 5 first years of the current experiment	1–1699 1700–1950 1950-start of the experiment	IS3NR	IS3FR	IS3SR

IS: initialization scenario, NR: No Relaxation, FR: Fast Relaxation, SR: Slow Relaxation.
M-W-Bl-F: Low yield wheat-barley-fallow 'maggese' rotation typical of roman and middle-age agriculture and meadow.
M-W-Bl: Low yield wheat-barley-meadow.
Moderate organic and inorganic fertilization, low tillage intensity were applied in all scenarios without irrigation.

2.3.3. Relaxation procedure

The relaxation procedure consisted of shifting (or not) the simulated SOC stocks at the end of the initialization, until they matched the SOC observed at the beginning of our experiments. The first modality (NR) consisted of leaving SOC pool sizes unchanged, at the end of initialization. The second technique was the fast relaxation (FR) which was adapted from the 'relaxed assumption' (Carvalhais et al., 2008) to the passive SOC pool of the CENTURY model V.4 (Hashimoto et al., 2011). This procedure consisted of scaling active, slow and passive carbon and nitrogen pools instantly at the end of the initialization period to reach the level of SOC stock measured at the beginning of the experiment while keeping the C to N ratio unchanged. The slow relaxation (SR) procedure consisted of extending relaxation during the final phase of the initialization period for hundreds of years (Hashimoto et al., 2011). In our study, we adjusted the total SOC while keeping the relative pools size (*i.e.*, for each pool i, the ratio between SOC stocks in pool i and total SOC stocks) unchanged at the final stage of initialization for three hundred years. In these pools, N was adjusted in order to keep the C to N ratio unchanged. Hashimoto et al. (2011) reported that this procedure enables a smoother transition from the spin-up run to the subsequent model run, which could avoid simulation artifacts induced by feedbacks from soil nitrogen to plant growth as well as complex interactions between soil carbon and nitrogen pools.

2.4. CENTURY model validation

The CENTURY model simulation results were thoroughly evaluated using several statistical criteria based on the comparison of observed and simulated data as is recommended by Bellocchi et al. (2010), under all initialization scenarios for each LTE/treatment. Validation was performed on the absolute (SOC_{abs}) and SOC stock change (ΔSOC) measurements. SOC_{abs} represented the total stock measured at each date and ΔSOC is calculated as the SOC_{abs} values minus SOC stock at the beginning of the experiment. ΔSOC was calculated to avoid the effect of mismatch between the predicted and observed SOC values with the NR scenarios.

2.4.1. Assessing overall CENTURY performance under initialization scenarios

The statistical criteria were as follows:

The mean prediction error (*MPE*),

$$MPE = \frac{1}{n}\sum_{i=1}^{n}(S_i - O_i) \tag{1}$$

where S and O represent the simulated and observed values, respectively, and n represents the number of observed-simulated pairs.

The root mean square prediction error (*RMSPE*), which estimates the magnitude of the model error, with small values indicating better model performance, was expressed as:

$$RMSPE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(S_i - O_i)^2} \tag{2}$$

The coefficient of determination (R^2), measuring the strength of the linear relationship between predicted and observed values and informing us about the dispersion was calculated as follows:

$$R2 = \left[\frac{\sum_{i=1}^{n}(S_i - \bar{S})(O_i - \bar{O})}{\sigma_S\sigma_O}\right]^2 \tag{3}$$

where $\bar{S}$ and $\bar{O}$ are the means of simulated and observed values, respectively, and σ_S and σ_O are the empirical standard deviations of the observed and simulated values, respectively.

Another widely used statistical criterion is the Nash-Sutcliffe efficiency (*NSE*), which measure agreement between simulated and observations values and ranges from -Inf to 1. The closer to 1 this value is, the more accurate the model is, with 1 corresponding to a perfect match of modeled and to the observed data. A value *of zero* indicates that the model is not performing better than the mean of observations and negative values, indicating that the observed mean is better than the model (Nash and Sutcliffe, 1970). This was calculated as follows:

$$NSE = 1 - \frac{\sum_{i=1}^{n}(S_i - O_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \tag{4}$$

2.4.2. Decomposition of CENTURY error

The relationship between predicted and observed SOC stocks was examined through the variations of CENTURY errors (*i.e.*, SOC_{abs} - simulations and ΔSOC - simulations) in response to different factors explained hereafter. We considered linear mixed effect models with varying intercept $\boldsymbol{\alpha_i}$ and slope $\boldsymbol{\beta_i}$ coefficients. Thus, for every observation i (*i.e.* CENTURY error), the response is described generically as:

$$\begin{cases} \boldsymbol{y_i} \sim \mathcal{N}(\boldsymbol{\mu_i}, \boldsymbol{\sigma_{ind}}) \\ \boldsymbol{\mu_i} = \boldsymbol{\alpha_i} + \boldsymbol{\beta_i}.\ \ \boldsymbol{t(i)} \end{cases} \tag{5}$$

For each combination of initialization scenario and treatment, the time variable (in years) was centered to facilitate the interpretation of the error model's intercept. In addition, the intercept $\boldsymbol{\alpha_i}$ was set to 0 for ΔSOC. The variation in the intercept and slope coefficients was split among different sources. Namely, the initialization scenarios decomposed in relaxation and management, the LTE, the treatment and their interactions (*i.e.*, factors). The linear mixed effect models consider time to be a fixed effect and random effects were the initialization scenarios (decomposed in relaxation and management), the LTE, the treatment and their interactions. We conducted a variable selection procedure (results not shown) by fitting alternative models by Maximum Likelihood considering the results of Likelihood Ratio Tests and the Akaike Information Criterion. For every observation i from LTE $s(i)$, with treatment $p(i)$ and initialization strategy given by management $m(i)$ and relaxation $r(i)$, the selected error's model 1 for SOC_{abs} was:

$$\begin{cases} \quad = \boldsymbol{\alpha_0} + \boldsymbol{\alpha_{p(i)}} + \boldsymbol{\alpha_{m(i),r(i)}} + \boldsymbol{\alpha_{m(i),r(i),s(i)}} + \\ \quad \boldsymbol{\alpha_{m(i),r(i),p(i)}} \\ \boldsymbol{\alpha_i} \quad = \boldsymbol{\beta_0} + \boldsymbol{\beta_{p(i)}} + \boldsymbol{\beta_{m(i),r(i),s(i)}} + \boldsymbol{\beta_{m(i),r(i),n(i)}} \\ \boldsymbol{\beta_i} \quad \sim \mathcal{N}\left(\boldsymbol{0}, \boldsymbol{\sum_p}\right) \\ (\boldsymbol{\alpha}, \boldsymbol{\beta})'_{\boldsymbol{p}} \\ \boldsymbol{\alpha_{m,r}} \quad \sim \mathcal{N}\left(\boldsymbol{0}, \boldsymbol{\sum_p}\right) \\ (\boldsymbol{\alpha}, \boldsymbol{\beta})'_{\boldsymbol{m,r,s}} \\ (\boldsymbol{\alpha}, \boldsymbol{\beta})'_{\boldsymbol{m,r,p}} \sim \mathcal{N}\left(\boldsymbol{0}, \boldsymbol{\sum_{mrs}}\right) \\ \quad \sim \mathcal{N}\left(\boldsymbol{0}, \boldsymbol{\sum_{mrp}}\right) \end{cases} \tag{6}$$

and the selected error model 2 for ΔSOC was

$$\begin{cases} \boldsymbol{\alpha_i} = \boldsymbol{0} \\ \boldsymbol{\beta_i} = \boldsymbol{\beta_0} + \boldsymbol{\beta_{m(i)}} + \boldsymbol{\beta_{r(i)}} + \boldsymbol{\beta_{s(i)}} + \boldsymbol{\beta_{p(i)}} + \boldsymbol{\beta_{m(i),s(i)}} + \\ \quad \boldsymbol{\beta_{m(i),p(i)}} + \boldsymbol{\beta_{r(i),s(i)}} + \boldsymbol{\beta_{r(i),p(i)}} + \boldsymbol{\beta_{m(i),r(i)}} + \boldsymbol{\beta_{m(i),r(i),s(i)}} \\ \boldsymbol{\beta_.} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\sigma_.}) \end{cases} \tag{7}$$

We checked and respected the normality of the predicted random effects and residuals as well as the stability of the estimates obtained from different models. We fitted all the models using the R package *lme4* (Bates et al., 2015), and the final results were based on a restricted log-likelihood (REML) estimation of variance components. We quantified the contribution of the factors to the total variance of CENTURY errors by generating sampling distributions using a bootstrap procedure based on 500 replicates with resampling using the R package *boot* (Canty and Ripley, 2016; Davison and Hinkley, 1997). The derived bootstrapped samples were then used to determine the difference between the most important variance components. All analyses were performed using the *R* 3.1.2 statistical software (R Core Team, 2016). The R code used for statistical analysis is available in the Appendix B.

3. Results

3.1. Simulated carbon stocks and pool sizes

3.1.1. Over the initialization period

During the initialization period, scenario managements strongly influenced the predicted SOC dynamics due to the differences in C inputs. As expected, the simulated total SOC stocks were different between LTEs with similar scenarios due to various intrinsic soil characteristics and the climate. In all scenarios, where each management was maintained for at least 1700 years (*i.e.*, first initialization period), the SOC active and slow pools reached equilibrium. The passive pool approached but did not reach equilibrium, because of its long mean residence time and weather inputs, which were not constant. The temporal dynamics of active, passive and slow SOC pools over the first 1700 years of the initialization period for the LTE Feucherolles treatment BIO are presented in Fig. 1. This figure gives a general picture of the SOC pools dynamics in response to various initialization scenarios managements and shows different equilibrium states for the same LTE.

3.1.2. At the end of the initialization period

Except for the Hessange LTE, the measured SOC stocks, in all LTEs, at the beginning of the experiments in the biologically active plowed layer (*ca.* 28 cm) ranged between 37.96 Mg ha^{-1} and 45.24 Mg ha^{-1}, with a C/N ratio ranging from 12.2 to 8 (Table 3). These values were in line with the usual observed values of French agricultural soils (Martin et al., 2011; Meersmans et al., 2012a, b; Mulder et al., 2015), which indicated that these LTEs had probably been under cropland management for several decades before the start of experiments. The predicted SOC stocks were close to the measured values at the end of the initialization period in NR scenarios in 4 of 6 LTEs (*i.e.*, Saint-Aoustrille, Auzeville, Boigneville and Feucherolles), suggesting that historical C

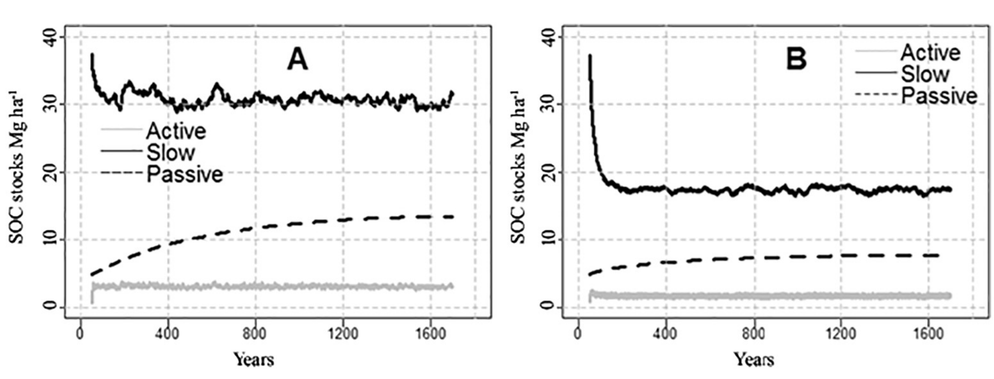

Fig. 1. Dynamics of simulated active (grey line), slow (black continued line) and passive (black dashed line) soil organic carbon pools during the first initialization period (1–1700 yr): A: for the initialization scenario IS1 and B: for the initialization scenarios IS2 and IS3 for the Feucherolle long term experiment.

Table 3
Total simulated soil organic carbon stocks after initialization for the no relaxation scenarios and observed soil organic carbon stocks at the beginning of the study, averaged by site over all treatments.

	Observed	Total OC stock (Mg ha^{-1})	Simulated scenarios	
Sites		IS1	IS2	IS3
Saint Aoustrille	41.42	50.22	40.12	42.93
Auzeville	37.96	31.37	38.74	34.68
Boigneville	42.33	28.68	43.20	34.68
Feucherolles	42.93	49.16	48.49	46.29
Hessange	75.30	99.93	54.45	58.44
Tartas	45.24	26.06	16.68	21.83

IS: Initialization scenario.

Table 4
Means and ranges of soil organic carbon pools (active, slow and passive) sizes expressed as a percentage of total organic carbon stock at the end of initialization scenarios.

Scenarios	SOC Pools proportions (%)					
	Active		Slow		Passive	
	Mean	Range	Mean	Range	Mean	Range
IS1NR	5.31	3.26–6.84	56.27	48.17–61.96	32.14	27.36–39.40
IS1FR	5.54	2.28–9.84	56.28	45.43–62.89	32.18	25.84–41.27
IS1SR	4.37	1.18–6.53	58.61	51.98–64.01	34.08	27.32–44.43
IS2NR	5.63	3.85–6.58	63.45	58.40–67.09	24.85	19.54–31.10
IS2FR	5.53	1.64–7.65	63.96	57.59–71.89	25.07	21.16–32.19
IS2SR	5.72	2.55–7.75	64.16	60.13–68.76	25.59	21.10–33.53
IS3NR	5.58	3.12–7.40	62.31	55.37–68.94	25.07	15.25–34.93
IS3FR	5.39	2.35–9.33	63.36	55.18–67.30	25.41	18.51–35.59
IS3SR	4.62	1.42–6.71	65.32	57.83–71.68	27.02	20.20–38.07

IS: initialization scenario, NR: No Relaxation, FR: Fast Relaxation, SR: Slow Relaxation.

input levels and mineralization were likely approached. The difference between observed and predicted SOC stocks for the four LTEs mentioned above, ranged from -0.87 Mg ha^{-1} to 13.65 Mg ha^{-1} (Table 3). Meanwhile, this difference exceeded 16 Mg ha^{-1} for Hessange and Tartas LTEs, and even reached 24.64 Mg ha^{-1} lower than the observed SOC stocks, for the scenario IS1 at the Hessange LTE. It is likely, that these LTEs were under land use that differed from the initialization scenarios. At the end of the initialization period, the SOC pool sizes varied among initialization scenarios and LTEs due to different soil characteristics, such as clay content and different climatic contexts. The mean average active pool sizes were close among initialization scenarios with a mean value of 5.3% of total SOC stocks (Table 4). The slow pool represented the biggest proportion of SOC stocks, in all scenarios, with an average value of 61.5%. The highest values of 63.66% and 63.85% were recorded for IS2 and IS3, respectively, and the lowest values were observed in IS1 scenarios (57.1%). Conversely, the passive pools proportions were higher in IS1 scenarios (32.8%) compared to the initialization scenarios IS2 (25.1%) and IS3 (25.8%) (Table 4).

3.2. Overall CENTURY model performance

3.2.1. CENTURY model evaluation

The examination of the CENTURY model performance, with estimated C inputs being adjusted, was performed, at first, using selected statistical criteria calculated based on the comparison of the simulated and observed absolute (SOC_{abs}) and SOC stocks changes (ΔSOC) for the *entire* experiments period (Table 5). The CENTURY model, which was initialized with the various scenarios considered, yielded satisfactory results when the predicted SOC_{abs} stocks were validated with global performance statistical criteria (*i.e.*, R^2, MPE, RMSPE, NSE computed with all LTEs considered). The R^2 (Eq. (3)) values ranged between 0.50 and 0.75. Only the NR scenarios showed limited performance (*e.g.*, IS1NR with a NSE value of -1.35 and IS2NR with a R^2 value of 0.48). The highest R^2 value was recorded for the IS2SR scenario (Table 5). A similar trend was observed for the ΔSOC but all performance indexes exhibited lower or equal (in case of relaxation for MPE and RMSPE) values compared to those of SOC_{abs}. The MPE values (Eq. (1)) for SOC_{abs}, for the entire experiment period ranged between 1.33 Mg ha^{-1} and 5.32 Mg ha^{-1}. The lowest and highest values were recorded in IS2SR and IS1NR, respectively. When the ΔSOC was considered for the same period, these values dropped slightly for the NR scenarios but were similar for the two relaxation procedure scenarios because we started with a perfect match between predicted and simulated SOC stocks. Furthermore, MPE values, for the NR scenario, remained above those of the relaxation scenarios, (*i.e.*, FR and SR), *except for IS2FR*. The RMSPE values (Eq. (2)), indicating the magnitude of the CENTURY error, were moderate compared to the total SOC stocks and their confidence intervals. The lowest value was 6.22 Mg ha^{-1} (13.1% of the initial average total SOC stock for all LTEs) for IS2SR, and the highest value reached 15.24 Mg ha^{-1} (32.1% of the initial average total SOC stock for all LTEs) for IS1NR. The NSE (Eq. (4)) values were low in the NR scenarios compared to the fast and slow relaxation scenarios for the variables SOC_{abs} and ΔSOC for the whole period. When these two variables were considered, the best NSE values were observed for the IS2SR (0.61 and 0.23 for SOC_{abs} and ΔSOC, respectively) (Table 5). The examination of all statistical criteria, which provided an assessment of the average performance of the model and initialization procedure indicated three major results: i) CENTURY performance was only slightly sensitive to initialization scenario managements and sensitivity depends on the output variable studied (SOC_{abs} *vs.* ΔSOC), ii) the best initialization scenario regarding CENTURY model performance was the IS2SR corresponding to the management reported by Lugato et al. (2014b) with the use of the slow relaxation procedure, as described by Hashimoto et al. (2011), and iii) the fast relaxation procedure did not generate an unstable CENTURY model behavior for the first years of simulation compared to the slow relaxation procedure.

3.2.2. CENTURY model error variation analysis

In the second step of the CENTURY performance evaluation, we examined the contribution of different factors (*i.e.*, relaxation procedure, and management of initialization scenarios, time, treatment/LTE and their interactions) to the variation of CENTURY errors (*i.e.*, simulated - observed SOC values) of the SOC_{abs} and ΔSOC, using linear mixed effect models (Eq. (6) and Eq. (7), see materials and methods section).

The evolution of CENTURY errors for SOC_{abs} over time and prediction of the fitted statistical models for all LTEs/treatments are presented in Fig. 2. This figure shows that the treatments (*i.e.*, agricultural practices) and the interaction between initialization scenarios and LTE factors had the greatest contribution to the total variance of CENTURY errors. This was confirmed by the examination of error model 1 intercepts results (Fig. 3A) showing that the treatment and initialization scenarios and LTE interaction contributed by 45.2% and 34.2%, respectively, to the total CENTURY error. The contribution of management and relaxation components of initialization scenarios remained limited, with values lower than 5.9% whereas the scenario and treatment interaction reached 9.3%. To examine the difference between the two most important factors that affect CENTURY error, we bootstraped the statistical model and found that the variance due to the treatment was 70.4% more likely to be greater than the variance due to the interaction of the initialization scenario and LTE (see Appendix A). The analysis of the error of the statistical model 1 slope, indicating the temporal effect of factors on the CENTURY error variance, showed a higher impact of the treatment with 98.8% of the total errors variance (Fig. 3A). The contributions of the interaction of scenario and LTE and scenario and treatment were very low, up to 1%, thus showing little impact of the initialization scenario on the temporal evolution of

Table 5
Main statistical criteria for CENTURY model evaluation for all experiments.

	Statistical criteria	Scenarios								
		IS1NR	IS1FR	IS1SR	IS2NR	IS2FR	IS2SR	IS3NR	IS3FR	IS3SR
SOCabs *Vs.* SOCsim	R^2	0.54	0.64	0.68	0.48	0.65	0.75	0.56	0.68	0.72
	MPE	5.32	3.76	3.93	2.72	2.62	1.33	2.16	3.06	3.10
	RMSPE	15.24	7.88	7.58	8.35	7.38	6.22	8.67	7.14	6.76
	NSE	− 1.35	0.37	0.42	0.3	0.45	0.61	0.24	0.48	0.54
ΔSOC *Vs.* SOCsim	R^2	0.12	0.23	0.28	0.1	0.23	0.36	0.17	0.29	0.35
	MPE	4.33	3.76	3.93	2.45	2.62	1.33	3.66	3.06	3.10
	RMSPE	8.69	7.88	7.58	8.27	7.38	6.28	7.95	7.14	6.76
	NSE	− 0.51	− 0.24	− 0.15	− 0.37	− 0.09	0.23	− 0.26	− 0.02	0.09

IS: initialization scenario, NR: No Relaxation, FR: Fast Relaxation, SR: Slow Relaxation.
R^2: The coefficient of determination, MPE: The mean prediction error (Mg ha^{-1}), RMSPE: The root mean square prediction error (Mg ha^{-1}), NSE: The Nash-Sutcliffe efficiency. SOC_{abs} represents the total soil organic carbon stock measured at each date, ΔSOC is calculated as the SOC_{abs} values minus SOC stock at the beginning of the experiment and SOCsim represent the simulated SOC values.

CENTURY errors.

We also examined the impacts of the factors mentioned above on ΔSOC CENTURY error over time using the model 2 error. In this case, ΔSOC *was* null, as was the measured SOC at the beginning of the experiments. Thus, the intercept was null and was not considered in the analysis. We noticed an important contribution of the LTE by approximately 95% of the total CENTURY error variance, whereas the treatment contributed by 3.9% and other factors contributed less than 1% (Fig. 3B).

4. Discussion

4.1. SOC pools distribution after initialization

The CENTURY model, which was run for the first initialization period (*i.e.*, approximately 1650 years), allowed active and slow SOC pools to reach equilibrium state and even allowed the passive pool to approach this state in some treatments. However, depending on the scenario management for the same LTE/treatment, different equilibrium states were obtained (*i.e.*, equilibrium reached with different SOC stocks and pools sizes distribution). These results showed that the reached equilibria do not necessarily, neither represent the actual LTE SOC level, nor do they guarantee better model simulations. Similar results of multiple possible equilibria, as produced by different initialization procedures, were also found in hydrological models (Ajami et al., 2015). The choice of an equilibrium state will certainly influence the optimization of potential decomposition rates (*i.e.*, when the passive pool is very high, its potential decomposition rates will increase and *vice versa*). Thus, various combinations of calibrated model parameters can fit equally well with the same observed total soil C dynamics, leading to equifinality issue (Luo et al., 2015). To ovoid this issue, the internal consistency of model outputs should be checked, and model predictions could be constrained by preventing unrealistic parameters combinations. CENTURY, similar to the vast majority of models simulating SOC dynamics, uses the mathematical formalism of linear dynamical systems (Manzoni and Porporato, 2007; Luo and Weng, 2011), which tends to reach equilibrium in the long term. Furthermore, it is difficult to disentangle the effects on SOC dynamic simulation between the crop management and/or climate from the drift due to CENTURY formalism. For predictions over few years or decades and if the passive

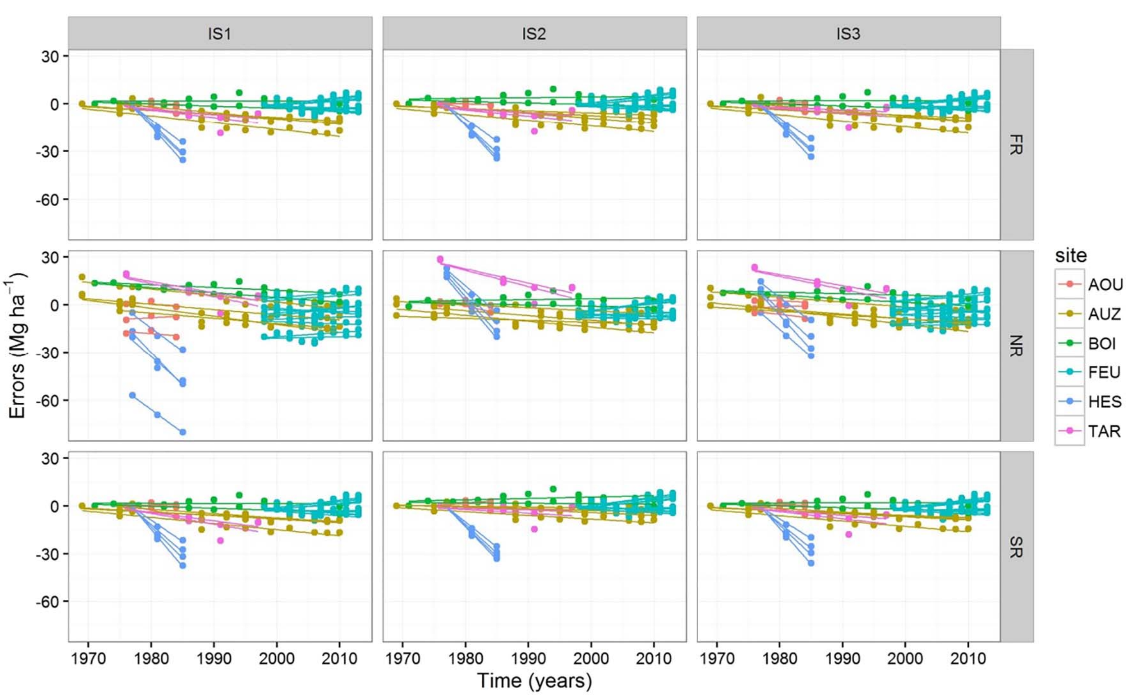

Fig. 2. CENTURY model errors (simulated minus observed SOC values (Mg ha^{-1})) evolution over time for all initialization scenarios and all long term experiment/treatments: AOU: Saint Aoustrille, AUZ: Auzeville,BOI, Boigneville, FEU, Feucherolles, HES: Hessange, TAR: Tartas. Circles and lines represent CENTURY errors and the fitted statistical model, respectively.

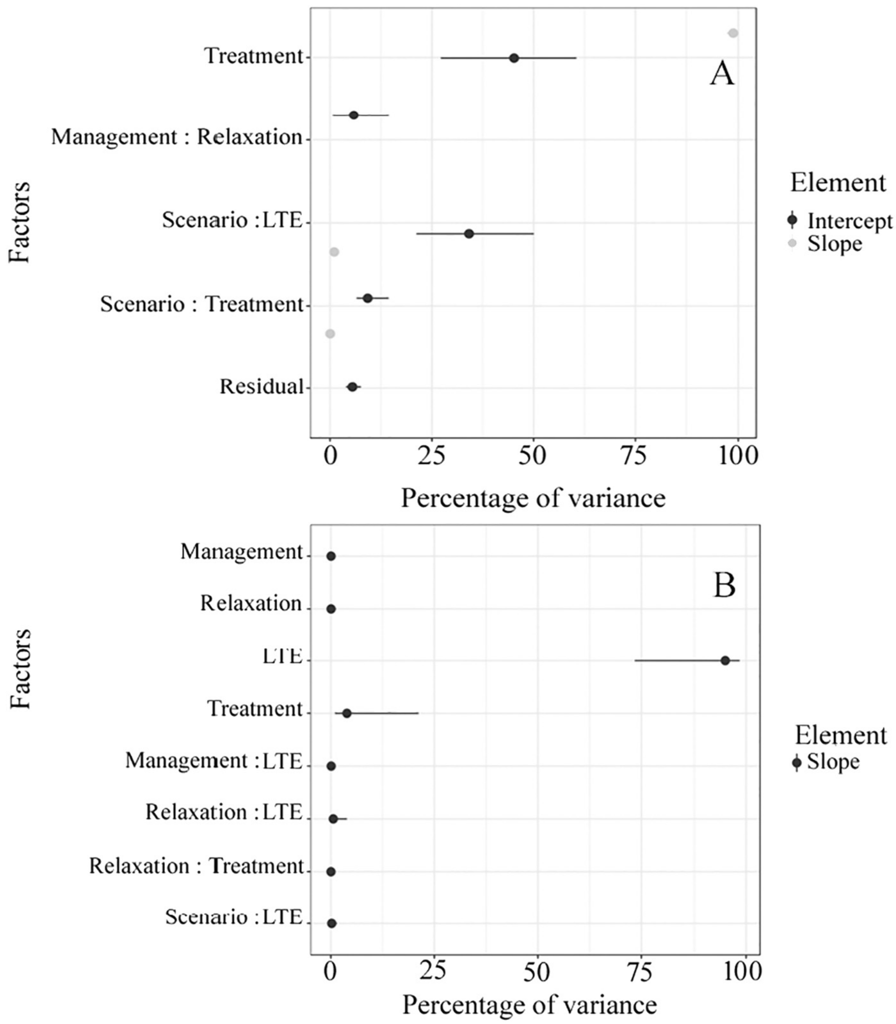

Fig. 3. Contribution of factors: treatment, long term experiment (LTE), initialization scenarios and their second-order interactions to the total explained variance of CENTURY model errors A (simulated minus observed SOC values) and B (simulated minus observed ΔSOC values). Black and grey circles represent the contribution of the factors to the variance related to the intercept and the slope, respectively, expressed as percentage of variance. Horizontal lines represent the bootstrapped 95% (percentile) confidence interval of the population.

pool has the largest pool size, this is likely not a significant issue because the dynamic is likely controlled by the short-term effect of the environmental drivers and the plant production. However, for long-term predictions (one or several centuries), the drift may become not negligible. In our study, when all scenarios were considered, there were small differences in the SOC pools depending on scenario initialization, but overall, we observed similar SOC pool distribution patterns. The slow pool represented the biggest proportion of SOC stocks, with the average values ranging from 56.2% to 65.3%. This consistent pattern might explain the relatively low difference in CENTURY model performance between relaxed scenarios (*i.e.*, FR and SR) when all LTEs are considered. Furthermore, our results did not show an unstable transient period after fast relaxation compared to *the* slow procedure of initialization scenarios. *This result was in contradiction to* the findings reported by Hashimoto et al. (2011). This *contradiction* may be explained by the relatively close *values of* observed and simulated SOC stocks at the end of initialization and thus, the relaxation effect became minimal. Nevertheless, the relaxation procedure has some shortcomings due to the uncertainty *of* measured SOC stocks induced by various factors (*e.g.*, carbon analysis methods, spatial representativeness of samples, inaccuracy of bulk densities and depth measurements). Schrumpf et al. (2011) examined the contribution of different sources of uncertainties (*i.e.* organic carbon concentration, bulk density and fine earth fraction) to the overall SOC stocks variance, at 12 CarboEurope LTEs under various climate, land use and soil types. The authors reported different contributions of these sources and found that the bulk density or the fine earth fraction were the most important contributors to the SOC stock variability in topsoil layers of croplands, whereas the relative importance of organic C concentration grew with depth (*i.e.*, from 36 ± 13% in the 0–5 cm layer to 73 ± 19% at 50–60 cm soil depth). This uncertainty could increase when scaling up SOC stocks from field to a larger scale, as reported by Goidts et al. (2009) in Belgian soils. In our study, the field spatial representativeness for all LTEs was considered with at least three soil sample replicates for each treatment. Furthermore, bulk densities were measured along the measurement of soil C content to calculate the SOC stock. The variance in measured initial SOC stocks was moderate, with confidence interval values not exceeding 18% with respect to the total initial SOC stock. The lowest value of 0.38% was observed at the Boigneville LTE. Further investigation is required to quantify the uncertainty of CENTURY model predictions induced by the uncertainty in SOC stock measurements at the beginning of the experiment. Few studies have addressed this issue, which has a direct impact on initial SOC values in the case of relaxation. Luo et al. (2016) constrained the APSIM model with the measurements of SOC stocks, including replicates to estimate a posterior distribution of selected model parameters (*i.e.*, the potential decomposition rate of the humic C pool and the amount of the recalcitrant C pool in total soil C). They suggested that, over long periods (*i.e.*, 100 years), the uncertainties induced by model parameterization (*i.e.*, several parameter estimation methods are tested) are larger than those induced by observations.

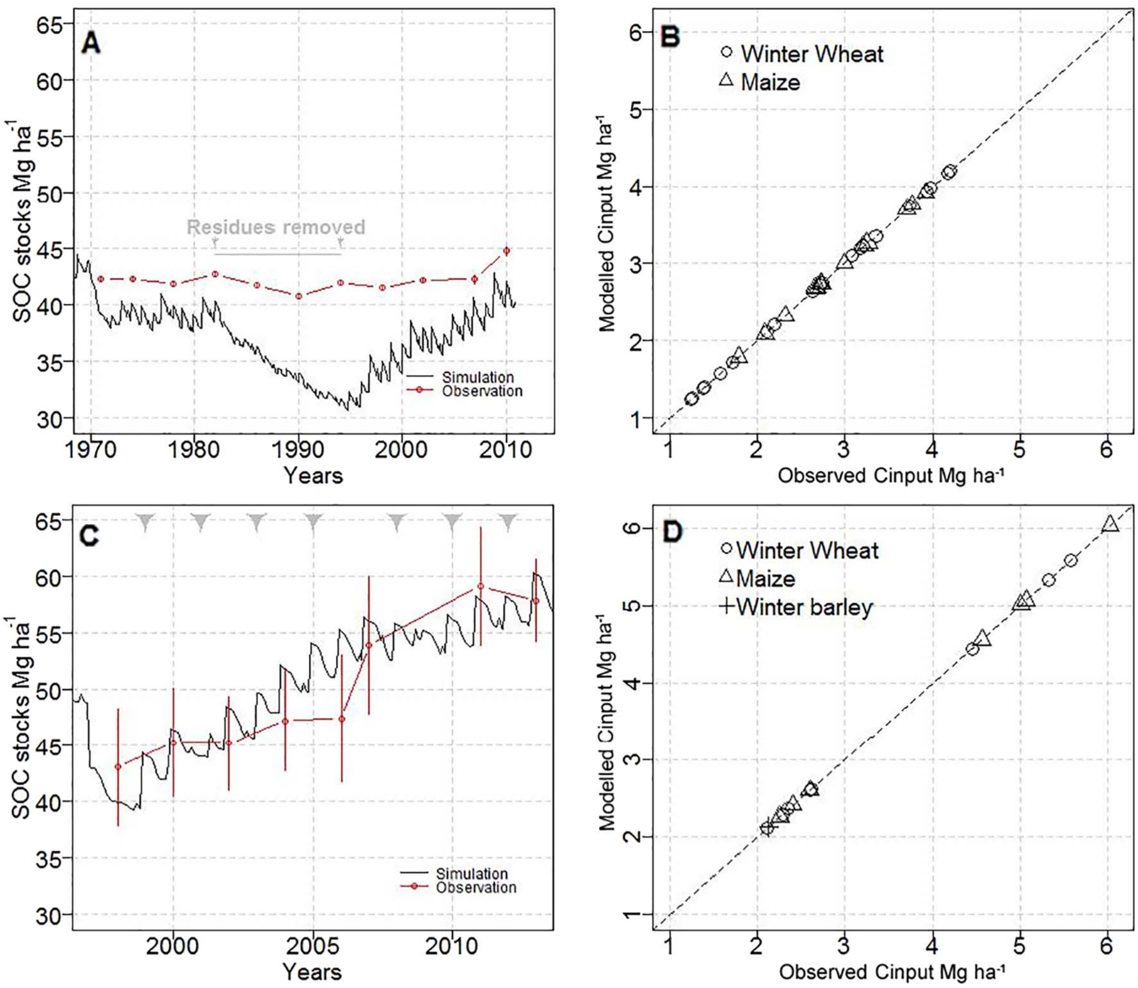

Fig. 4. Observed (red lines) and simulated (black lines) soil organic carbon stocks (SOC) changes, in the plowed layer about 28 cm), for two long term experiments (LTEs) Boigneville (A) and Feucherolles (C) farm yard manure (FYM) treatment. Error bars (vertical red bars) are the confidence intervals of SOC observations and grey arrows represent the residues removing events (continuous twelve years for Boigneville and once every two years for Feucherolles). The correspondent modeled and observed (estimated based on yields) above and below ground C inputs derived from crops are indicated in (B) for Boigneville and (D) for Feucherolles (FYM) LTEs. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4.2. Overall CENTURY model evaluation

With our chosen initialization scenarios, the CENTURY model with forced C inputs showed fair results overall for SOC_{abs} predictions (when assessed with average performance statistical criteria such as R^2, MPE, RMSPE and NSE). However, the ability of Century to reproduce SOC changes was by far poorer. This resulted in a globally fair to poor performance that depended mainly on the initialization scenario. For some LTEs, such as those with organic amendments, CENTURY satisfactorily simulated SOC changes. These findings are in accordance with many studies that show satisfactory simulation results, since the CENTURY model is well validated and widely applied for LTEs in *the context of* multiple agroecosystems context (*e.g.*, in the USA (Metherell et al., 1993; Parton and Rasmussen 1994), Canada (Liang et al., 1996; Smith et al., 2000), Sweden (Paustian et al., 1992), and Australia (Carter et al., 1993; Probert et al., 1995)). However, CENTURY failed to simulate the effect of crop residues harvested at the Boigneville LTE (Fig. 4A), likely due to an overestimation of potential decomposition rate of structural and metabolic surface SOC pools, even with adjusted crop derived C inputs (Fig. 4B). Another possibility is that the ratio that we used to estimate the belowground C input was inaccurate for some crops, yielding an over- or underestimation of C inputs. Our findings were in line with those of Necpálová et al. (2015), who calibrated of 67 DAYCENT model parameters by using an inverse modelling procedure. The simulated SOC was found to be very sensitive to the nature of residues, essentially the C/N ratio and the lignin content. This may explain the widening of the gap between measured and predicted SOC stocks over time. Residues removed treatment was, also applied in the Feucherolles LTE, once every two years (Fig. 4C). However, the SOC simulation quality was not affected in this LTE, as much as *the* Boigneville *LTE*, likely because of the important organic amendment inputs that could mask this effect and the higher crop derived C input (Fig. 4D). Campbell et al. (2014) found similar results with the DAYCENT model (*i.e.*, the daily version of CENTURY), which showed a clear bias of estimating SOC loss with conventional tillage and residue removal. CENTURY also failed to simulate SOC stocks and dynamics of the Hessange LTE, where the crop rotations included Rapeseed and Sunflower crops.

4.3. CENTURY model errors

The CENTURY model error analysis for the full data set allowed us to assess the overall impacts of initialization scenarios on SOC simulations, as well as the effects of agricultural practice. The results showed little effect of initialization scenarios on CENTURY simulation performance when scenarios were considered individually, but the second-order interaction effect with LTE (*i.e.*, agricultural practices) was important for predicting SOC levels (*i.e.*, the SOC_{abs} variable). However, initialization methods did not have a significant impact, alone or in interaction with other factors, on CENTURY error when predicting SOC changes (*i.e.*, the deltaSOC variable). This may be due to the fact that the initial SOC levels were not constrained by the observed values for the NR scenarios, which may have induced a variation in the errors on initial SOC levels. The Intensity of these variations depends on the LTE characteristics and the management scenario. These variations were high compared to those caused only by SOC dynamics during the LTE simulated periods of time, hence the contribution of scenario-related factors to SOCabs errors. When considering DeltaSOC, the impact of scenario on base levels vanished, because all DeltaSOC time series (simulated and observed) shared the same initial value, (*i.e.*, zero change at the starting date). These results show that the most important factors for explaining variance of deltaSOC errors are, by far, the LTE and the treatment. This emphasized the diversity of our LTEs in terms of soils, climate, agricultural systems and data quality, resulting in diverse model performance, independent of the initialization procedure. When we examined other studies that investigated the initialization effects on the performance of models simulating SOC decomposition, we found contradicting conclusions. For instance, Foereid et al. (2012) used different initialization methods for the DAYCENT model to predict changes in soil carbon for a range of soils, climates and land use across England and Wales during the period 1981–1999 and found that the predicted absolute rates of change in carbon content were sensitive to model initialization. Ogle et al. (2010) used the CENTURY model to estimate changes in SOC stocks and to upscale results from point locations to the entire US croplands during the 1990s, addressing uncertainties in model inputs and structure. They found that the most of the uncertainty was associated with the model structure (*i.e.*, algorithms and parametrization including initial values) and initialization procedure. Luo et al. (2015) applied the process-based PASIM model to 90 individual field experiments across the Australian cereal-growing regions to simulate and predict the SOC dynamics for 100 years. They reported that the *three* most important parameters contributing to the uncertainty in the projected SOC dynamics were 1) the microbial carbon use efficiency *with* the biggest impact, 2) the potential decomposition rate constant of humic organic matter (k_{hum}, day-1) and 3) the fraction of the humic carbon that is recalcitrant to decomposition (*finert*) corresponding to the passive pool in the CENTURY model. In contrast, Senapati et al. (2013) used the RothC model with different initialization methods to simulate the SOC dynamics for relatively undisturbed native grasslands in Australia under climate change at 12 LTEs. They found that when all LTEs and initialization methods were considered, the average maximum absolute differences in projected SOC stocks (*i.e.*, percentage of initial 2008 SOC stocks) and the average absolute variations throughout the projection period were very small 2.2 and 1.6%, respectively. These results suggest that projections of SOC under climate change are relatively insensitive to the model initialization methods. Overall, we argue that initialization contributes greatly to process-based models errors and uncertainty on SOC levels. We believe simply that this is due to principle of some of them (relaxation sets SOC levels to observed initial values). However, this contribution must be considered in interaction with the studied LTE/treatments. Some initialization procedures, especially those involving slow relaxation, seem to be on average, preferable to others. However, LTE and treatment characteristics have much more weight than do initialization scenarios alone.

5. Conclusion

We examined nine initialization scenarios (*i.e.*, three crop managements combined with three relaxation procedures, including no relaxation) and their impacts over time on CENTURY model simulations quality of SOC dynamics in six LTEs, across France, with 25 treatments. We showed that the CENTURY model had contrasting results for simulating SOC changes, when standard parameters and crop derived C inputs were adjusted. We found satisfactory results for the application of organic amendments and cropping systems but the CENTURY model failed to capture the effects of residue harvested treatments on SOC dynamics. Overall, two important results stemmed from our work First, the choice of initialization scenarios with their two components (*i.e.*, managements and relaxation procedures) have little effect on the quality of CENTURY SOC simulations quality, and this effect vanished almost completely when the changes in SOC errors were studied instead of studying errors in SOC levels only. The errors of the CENTURY model to reproduce SOC changes were highly variable and depended on characteristics of LTEs and treatment, possibly on observational data accuracy, rather than on the characteristics of initialization scenarios.

Data and code availability

The data of the long-term experiments, from this study are available in papers mentioned in the Materials and methods section and in the references. The process-based CENTURY model is available on request at https://www.nrel.colostate.edu/projects/century. (Registration not required). The R code used for statistical analysis is available in the Appendix B.

Competing interests

The authors declare that they have no conflicts of interest.

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Supplementary material. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.geoderma.2017.09.038.

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