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

Bassem Dimassi[a,*], Bertrand Guenet[b], Nicolas P.A. Saby[a], Facundo Munoz[c], Marion Bardy[a], Florent Millet[a], Manuel P. Martin[a,*]

[a] INRA, US InfoSol 1106, 45160 Ardon, France
[b] Laboratoire des Sciences du Climat et de l'Environnement, LSCE/IPSL, CEA-CNRS-UVSQ, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France
[c] INRA, UR AGPF 0588, 45160 Ardon, France

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ABSTRACT

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 FAOST-AT 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

* Corresponding author.
*E-mail addresses:* bassem.dimassi@inra.fr (B. Dimassi), manuel.martin@inra.fr (M.P. Martin).

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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-