



Modeling soil organic carbon evolution in long-term arable experiments with AMG model



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ABSTRACT

Reliable models predicting soil organic carbon (SOC) evolution are required to better manage cropping systems with the objectives of mitigating climate change and improving soil quality. In this study, data from 60 selected long-term field trials conducted in arable systems in France were used to evaluate a revised version of AMG model integrating a new mineralization submodel. The drivers of SOC evolution identified using Random Forest analysis were consistent with those considered in AMG. The model with its default parameterization simulated accurately the changes in SOC stocks over time, the relative model error (*RRMSE* = 5.3%) being comparable to the measurement error (*CV* = 4.3%). Model performance was little affected by the choice of plant C input estimation method, but was improved by a site specific optimization of SOC pool partitioning. AMG shows a good potential for predicting SOC evolution in scenarios varying in climate, soil properties and crop management.

1. Introduction

Soils are fundamental to many provisioning and regulating ecosystem services, the prediction of which requires improving our understanding of soil processes and their modeling (Smith et al., 2015; Vereecken et al., 2016). In agricultural systems, soil organic matter (SOM) plays a crucial role in soil structure, quality and fertility for crop production (Tiessen et al., 1994; Reeves, 1997). SOM also constitutes an important reservoir of carbon (C) whose dynamics can significantly impact the global C cycle (Heimann and Reichstein, 2008). Soil organic carbon (SOC) can act as a sink or source of atmospheric C and has therefore the potential of mitigating climate change by increasing C storage in agricultural soils (Paustian et al., 1997, 2016), leading to the recent “4 per mille” initiative (www.4p1000.org). Croplands, which are depleted in SOC compared to grasslands and forests (Smith, 2008; Poeplau et al., 2011), have a great potential for C sequestration (Lal and

Bruce, 1999; Smith, 2004).

SOC dynamics in arable systems is mainly driven by i) C inputs into soils from crop residues and organic amendments generating newly-formed SOM (Kuzyakov and Domanski, 2000; Mandal et al., 2007; Maillard and Angers, 2014) and ii) C outputs due to SOM decomposition and erosion. The unbalance between these two opposite fluxes determines soil C decline or accumulation. An accurate estimation of C inputs and the consideration of the relevant drivers of SOM mineralization and stabilization are therefore needed to better predict SOC stock evolutions, which are primarily under the influence of pedoclimatic conditions and agricultural practices (Stockmann et al., 2013; Dignac et al., 2017). SOC turns over slowly and variations in SOC stocks can only be reliably detected on the mid or long-term in most cases. There is consequently a need for long-term experiments (LTEs) to calibrate and validate mathematical models able to reproduce accurately SOC dynamics and reliably predict future SOC evolutions.

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Numerous and various soil biogeochemical models featuring different levels of complexity have been designed to simulate SOC dynamics (Falloon and Smith, 2000; Manzoni and Porporato, 2009; Campbell and Paustian, 2015). These models can be used to predict SOC stock evolution, better understand their driving factors and test methods and hypotheses regarding i) estimates of plant C inputs into soils (Taghizadeh-Toosi et al., 2016; Keel et al., 2017), and ii) mineralization of SOM and its partitioning into functional C pools (Zimmermann et al., 2007; Herbst et al., 2018). Among the diversity of soil C models, simple process-oriented models may have some advantages compared to more complex ones or organism-oriented models (Stockmann et al., 2013). They require a lower number of input variables and have been designed to simulate SOC evolutions with a reduced set of functions and parameters reflecting the main processes driving SOC dynamics. They can be applied to a larger number of experiments and/or over longer time and spatial scales. When correctly calibrated, they may represent a good compromise between complexity and reliability for general applications and could be used as decision support tools to help managing SOC in arable systems.

The aim of this study was to enhance the reliability of AMG, a simple model simulating soil C at annual time steps (Andriulo et al., 1999), in predicting SOC stock evolution in topsoils from arable cropping systems. AMG was previously shown to satisfactorily simulate the effects of straw residue export on SOC in various cropping systems and pedoclimatic conditions (Saffih-Hdadi and Mary, 2008) and the effects of alternative arable systems (Autret et al., 2016). It was also used as a tool for designing innovative cropping systems (Colnenne-David and Doré, 2015; Dufossé et al., 2016). In this work, we evaluated a revised version of AMG, in which was implemented a new model of SOM mineralization calibrated for the prediction of N mineralization in arable soils (Clivot et al., 2017). We hypothesized that the main identified driving factors of soil organic N mineralization could apply for the prediction of SOC mineralization due to a tight soil C and N coupling (Zaehle, 2013) and could also improve the modeling of SOC dynamics. We analyzed the impact of two major sources of uncertainty in SOC modeling using several methods related to i) estimation of aboveground (AG) and belowground (BG) plant C inputs and ii) partitioning of total SOC between active and stable pools, and the relevance of these methods for AMG model.

2. Material and methods

2.1. Experimental sites

In a first step, we compiled all the available LTEs carried out in arable cropping systems in France by research teams or extension services since 1970, in which SOC had been measured at several dates. They represented 455 treatments spread over 53 sites. We then selected the most reliable experiments by applying the following criteria: number of replicates ≥ 3 ; number of measurement dates ≥ 3 ; experiment duration ≥ 8 years; mean coefficient of variation of SOC measurements $\leq 10\%$; rock fragment content nil or measured. The selection leads to a reduced dataset of 60 treatments located in 20 sites (Fig. 1), covering however a large diversity of pedoclimatic conditions (Table S1), crop rotation types and practices (Table S2) representative of most French arable systems.

The field experiments were carried out between 1970 and 2015, lasting between 8 and 41 years (median value of 22 years) (Table 1). The mean annual temperature observed during the field trials ranged from 9.9 to 13.5 °C (median value of 11.0 °C). The annual precipitation ranged from 637 to 1285 mm (median 753 mm) and potential evapotranspiration from 637 to 947 mm (median 721 mm). The field trials exhibited contrasting soil physicochemical parameters. The clay content ranged from 43 to 308 g kg⁻¹ (median 214 g kg⁻¹), silt content from 95 to 781 g kg⁻¹ (median 528 g kg⁻¹), sand content from 12 to 791 g kg⁻¹ (median 140 g kg⁻¹) and CaCO₃ content of soils varied from

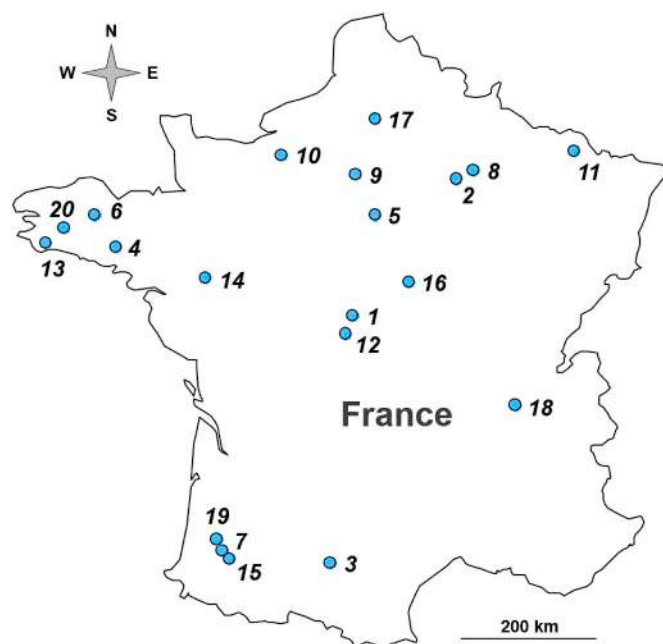


Fig. 1. Location of the 60 field trials distributed among 20 sites in France. The correspondence between site numbers and field-experiments is defined in Tables S1 and S2.

Table 1

SOC stock variations, mean climatic conditions and soil physicochemical parameters measured for the 60 field trials.

	Units	Min	Max	Median	Mean	SD
SOC stock variations						
Considered soil depth	cm	20	30	28	27	3
Initial SOC stock	t C ha ⁻¹	25.1	115.3	43.8	53.5	21.2
SOC stock changes (final-initial)	t C ha ⁻¹	-24.0	7.1	-1.2	-3.6	7.3
Experiment duration	yr	8	41	22	24	12
Annual SOC stock change rates	t C ha ⁻¹ yr ⁻¹	-1.01	0.45	-0.08	-0.20	0.33
Annual climatic conditions						
Mean temperature	°C	9.9	13.5	11.0	11.5	1.1
Cumulative Precipitation	mm	637	1285	753	840	220
Cumulative PET	mm	637	947	721	722	77
Precipitation-PET	mm	-290	595	37	117	252
Soil properties						
Clay	g kg ⁻¹	43	308	214	197	76
Silt	g kg ⁻¹	95	781	528	488	176
Sand	g kg ⁻¹	12	791	140	233	194
CaCO ₃	g kg ⁻¹	0	781	0	82	209
pH		5.6	8.3	6.8	7.0	0.9
C/N		7.8	13.0	9.1	9.4	1.1
Initial SOC content	g kg ⁻¹	7.2	32.9	14.1	15.8	6.8
Bulk density	g cm ⁻³	1.20	1.52	1.40	1.38	0.08
Rock fragment	%	0	39	0	7	10

PET: potential evapotranspiration, SOC: soil organic carbon.

0 to 781 g kg⁻¹ (median 0 g kg⁻¹). Soil pH varied between 5.6 and 8.3 (median 6.8). Bulk density ranged from 1.20 to 1.52 g cm⁻³ (median 1.40 g cm⁻³). Initial soil organic C (SOC) stocks in the topsoils (ploughed layer, 0–20 to 0–30 cm) varied widely, from 25 to 105 t C ha⁻¹ (median 44 t C ha⁻¹).

Cropping systems encountered in the 60 treatments were cereal-based rotations with legumes and/or oilseed crops (32% of the cropping systems), grain maize/winter wheat rotations (27%), rotations with silage maize (23%, including 3 out of 14 treatments in monoculture), grain maize monocultures (10%), cereals/sugarbeet rotations with

legumes and/or rapeseed (7%) and 1 treatment was a bare fallow soil. Winter cover crops were occasionally grown in 10 treatments (17%) on 3 different sites. Straw residues were regularly exported in 38% of the treatments and returned to soil in 62% of them. Exogenous organic matters (EOM) were applied as manure or slurry in 11 treatments (18%) from 5 different sites. Crops were grown with conventional N rate applications providing a positive N balance in most situations. Seven sites included variations in P or K fertilization rate but they did not reveal major effects on yield or aboveground plant biomass production. Conventional tillage with full inversion ploughing was conducted in all treatments except 6 treatments from the BOIG-site where soils were maintained under no-till. Past land use of the investigated sites was cropland except the 5 treatments from the KERB-site which were previously under sown grassland. Details on cropping systems can be found in Table S2.

2.2. Soil physicochemical analyses

For each field trial, top soil layers were sampled in 3–4 replicates on several occasions to determine soil physicochemical characteristics and SOC stocks. The sampling depth varied between 20 and 30 cm (median 28 cm), and was equal or greater than the greatest ploughing depth recorded during the study. For each soil characterization, several soil cores were collected and mixed together to obtain a representative composite sample. Particle-size distribution was determined on non-decarbonated soil samples using the pipette method according to NF ISO 11277. Soil CaCO_3 content was quantified by a volumetric method following NF ISO 10693 and soil pH was measured at a 1:5 soil/water ratio (NF ISO 10390). Soil bulk density (BD) was determined either by the cylinder method or the gamma radiation method (Blake, 1965) or estimated according to the soil pedological class. The determination of soil organic C (SOC) was performed by colorimetry after sulfochromic oxidation (NF ISO 14235). Soil organic N (SON) was quantified following NF ISO 11261, by using the Kjeldahl method after sulfuric acid digestion. In the later years, the dry combustion method was used to determine total C and N at some sites. The two different methods were shown to produce very close estimates of SOC and SON concentrations (Dimassi et al., 2014) and were therefore not distinguished later.

The SOC stock (QC , expressed in t C ha^{-1}) at the considered soil depth z (m) was calculated as follows (Poelau et al., 2017):

$$QC(z) = C \cdot z \cdot BD \cdot (1 - R_f) \cdot 10 \quad (1)$$

where C is the SOC content (g C kg^{-1}), BD is the bulk density of fine earth (g cm^{-3}) and R_f the volumetric fraction of rock fragments ($> 2 \text{ mm}$) unaccounted for in the analysis.

2.3. Climatic data

For each experimental site, mean annual air temperature ($^{\circ}\text{C}$) and annual cumulative precipitation (mm) and potential evapotranspiration (PET in mm, Penman, 1948) were calculated using daily data obtained from the closest weather station (the distance between the experimental sites and the weather stations varied from 0 to 55 km, on average 11 km).

2.4. AMG model

2.4.1. Model description

AMG is a model designed to simulate soil C dynamics at an annual time step (Andriulo et al., 1999; Saffih-Hdadi and Mary, 2008). The model considers three organic matter (OM) compartments: fresh OM (FOM) coming from crop residues or organic amendments which can be decomposed or humified, and SOM which is divided into active (C_A) and stable C pools (C_S). Humified FOM is allocated to C_A , which is affected by the mineralization process. C_S is considered completely recalcitrant to mineralization during the prediction time ($< 100 \text{ yrs}$).

AMG can be described by this set of equations:

$$QC = QC_S + QC_A \quad (2)$$

$$\frac{dQC_A}{dt} = \sum_i m_i h_i - kQC_A \quad (3)$$

where QC is the total SOC stock (t ha^{-1}), QC_A and QC_S are the C stocks of the active and stable C pools (t ha^{-1}) respectively, m_i is the annual C input from organic residue i ($\text{t ha}^{-1} \text{ yr}^{-1}$), h is its humification coefficient (the fraction of C inputs which is incorporated in SOM after 1 year) and k is the mineralization rate constant of the active C pool (yr^{-1}). The model allows simulating separately the C originating from C_3 or C_4 crops using ^{13}C natural isotopic abundance measurements (Appendix A).

2.4.2. SOC pool partitioning

In the default parameterization, the initial proportion of the stable pool (C_S/C_0) was set at 65% of total C for conditions of land use with a long-term arable history (Saffih-Hdadi and Mary, 2008). In the case of arable soils with a long-term grassland history, C_S/C_0 was assumed to be lower as suggested by Huggins et al. (1998) and was set by default at 40% of initial SOC content, this value corresponding to the lower limit of optimum values found earlier for simulating SOC evolutions with AMG (Saffih-Hdadi and Mary, 2008).

2.4.3. Environmental functions

In AMGv1, the mineralization rate k of the active C pool depends on climatic conditions and soil characteristics and is calculated using environmental functions as follows:

$$k_{AMGv1} = k_0 \cdot f(T) \cdot f(H) \cdot f(A) \cdot f(\text{CaCO}_3) \quad (4)$$

where k_0 is the potential mineralization rate (yr^{-1}), $f(T)$ is a function of mean annual air temperature ($^{\circ}\text{C}$) and $f(H)$ is a function used as a proxy to describe the effects of soil moisture. $f(H)$ is a function of the annual water inputs (precipitation and irrigation water) and PET. $f(A)$ and $f(\text{CaCO}_3)$ are reduction rate functions of clay and CaCO_3 contents on SOM mineralization, respectively.

In AMGv2, we implemented the model of SOM mineralization recently developed for the prediction of N mineralization in arable soils (Clivot et al., 2017), so that the mineralization rate k is calculated in this modified version following this equation:

$$k_{AMGv2} = k_0 \cdot f(T) \cdot f(H) \cdot f(A) \cdot f(\text{CaCO}_3) \cdot f(\text{pH}) \cdot f(\text{C/N}) \quad (5)$$

where $f(T)$, $f(H)$, $f(A)$ and $f(\text{CaCO}_3)$ are the same functions than in AMGv1, the parameter values of $f(A)$ and $f(\text{CaCO}_3)$ differing slightly between the two versions. In AMGv2, the additional functions $f(\text{pH})$ and $f(\text{C/N})$ describe the effects of soil pH (increasing function) and C:N ratio (Gaussian function) on SOM mineralization. The soil functions $f(A)$ and $f(\text{CaCO}_3)$ and their associated parameters in AMGv1 are similar to those used in the v8.5 and earlier version of the STICS model (Coucheny et al., 2015), while those in AMGv2 are corresponding to the mineralization model developed in Clivot et al. (2017), except the parameterization of $f(\text{CaCO}_3)$, which has been optimized independently using mineralized N data in chalky soils (unpublished data). The potential mineralization rate k_0 was the only parameter optimized with AMG for the calibration of each version of the model. All the functions and parameters are detailed in supplementary material (Appendix A).

2.4.4. Calculation of carbon inputs

We adapted to French experimental data the approach described in Bolinder et al. (2007) to calculate relative annual C allocation coefficients in the different plant parts in order to estimate aboveground (AG) and belowground (BG) C inputs from crops residues. Plant aboveground C was calculated according to measured dry matter yield (Y_p , expressed in $\text{t ha}^{-1} \text{ yr}^{-1}$) and mean harvest index (HI , grain to aerial biomass (including grain) ratio) obtained from a compilation of data from

French experiments. Plant C in straw and stubble (C_{SS}) was calculated using a C content of 0.44 g g^{-1} in the aboveground plant material (Redin et al., 2014):

$$C_{SS} = Y_P \cdot \frac{1 - HI}{HI} \cdot 0.44 \quad (6)$$

Aboveground C inputs (C_{AG}) depend on the fraction of C_{SS} (P_{SS}) that is returned to the soil:

$$C_{AG} = P_{SS} \cdot C_{SS} \quad (7)$$

P_{SS} value being equal to 1 when all crop residues are left in the field or lower than 1 when a part of C_{SS} is exported. P_{SS} values were determined for the different crops in case of straw residues export (P_{SE}) and correspond to the fraction of C_{SS} , represented by stubble and chaff, that is left to the soil. P_{SE} values for the different crops are reported in Table S3.

For BG input estimates, two C pools were calculated: 1) plant C in roots (C_R) and 2) plant C in extra-root material (C_E) which corresponds to organic matter deriving from root-turnover and root exudates. C_R for the different crops were calculated using shoot-to-root ratios (SR) compiled in Bolinder et al. (2007) and completed by French experimental data, assuming a C content of 0.40 g g^{-1} in the BG plant material (Boiffin et al., 1986), lower than in AG crop residues (Buyanovsky and Wagner, 1986):

$$C_R = \frac{Y_P}{SR \cdot HI} \cdot 0.40 \quad (8)$$

Extra-root C inputs were calculated following the assumption made by Bolinder et al. (2007):

$$C_E = 0.65 \cdot C_R \quad (9)$$

In order to estimate BG inputs, we used the asymptotic equation of Gale and Grigal (1987) to determine the cumulative BG input fraction ($BG_{F-Depth}$) from the soil surface to a considered depth (cm):

$$BG_{F-Depth} = 1 - \beta^{Depth} \quad (10)$$

where β is a crop-specific parameter determined using the root distributions for temperate agricultural crops reported in Fan et al. (2016). Calculated β values are reported in Table S3. The depth was set at 30 cm to calculate BG inputs (C_{BG}):

$$C_{BG} = BG_{F-30} \cdot (C_R + C_E) \quad (11)$$

Calculated BG inputs, expressed in t C ha^{-1} , were further corrected for site-specific considered depth (20–30 cm in this study) by the AMG model. Relative annual C allocation coefficients obtained for the crops encountered in our experiments are reported in Table S3. C inputs from exogenous organic matter (EOM) were calculated according to the amount of organic amendment applied and to measured C content conversion coefficients and were expressed in t C ha^{-1} .

2.4.5. Humification coefficients

Humification coefficients of AG crop residues were calculated as in the STICS model (Coucheney et al., 2015) using their specific average C/N ratio (Machet et al., 2017) and the functions and parameterization described in Justes et al. (2009), low C/N ratio of crop residues promoting humification. The calculated humification coefficients, ranging from 0.22 (for a C/N ratio of 82) to 0.31 (for a C/N ratio of 22) for the different crops, are reported in Table S3.

We assumed that root derived C contributed more to stored SOC than the same amount of C derived from AG crop residues (Balesdent and Balabane, 1996; Ghafoor et al., 2017; Kätterer et al., 2011). We calculated a value of 0.39 for the humification coefficient of BG inputs, both using the data of Balesdent and Balabane (1996) and Kristiansen et al. (2005) with ^{13}C tracing and root incubation experiments described in Justes et al. (2009). It corresponds to a relative contribution of BG material to humified C 26%–77% greater than that of AG

residues. This range is in accordance with the data compiled by Rasse et al. (2005) who found an average of 30% increase of humification coefficient for root compared to shoot material in incubation studies.

Humification coefficients of diverse EOMs were determined by soil incubations and inverse modeling in AMG simulations performed on field-experiments. They were used for the parameterization of EOMs applied into soils of this study. Humification coefficients used were 0.52 and 0.53 for bovine and pig manure respectively, and 0.50 and 0.15 for bovine and pig slurry, respectively (Bouthier et al., 2014).

2.5. Model simulations

2.5.1. Modeling steps

Prior to simulations of SOC stock evolutions with AMG model, we first used Random Forest (RF) regression analysis as a mean to identify relevant variables (Hapfelmeier and Ulm, 2013) driving SOC stock change rates in our experiments. SOC stock change rate, as the response variable, was calculated as the slope of the linear regression of SOC stocks against time in each trial. Selected input variables for the RF analysis were related to climatic conditions (mean annual temperature, cumulative precipitation and PET), soil characteristics (initial SOC stock, soil pH, C:N ratio, clay, silt, sand and CaCO_3 contents) and agricultural practices (frequencies in the rotation of straw residue export, bare fallow or winter cover crops and mean annual EOM applications). RF was run in R Software version 3.3.0 (R Core Team, 2016) using the *randomForest* package (Liaw and Wiener, 2002), the number of trees being set to $n_{tree} = 100,000$ to ensure convergence, while the other parameters were set to their default values. The performance in predicting SOC stock change rates by RF was compared with that obtained with the two model versions (AMGv1 and AMGv2) against the database. After this first step in which we analyzed SOC stock change rates, we focused on the simulations of soil C stocks with AMG model. The quality of prediction of AMGv1 and AMGv2 was compared to the SOC evolution measured in the 60 field trials. Using AMGv2, we evaluated the effects of alternative methods for estimating plant C inputs (2.5.2) and for setting the initial stable C pool proportion (2.5.3). We also performed a sensitivity analysis of AMGv2 outputs to the different input variables (see part 2.6.2).

2.5.2. Assessment of plant C inputs

Using AMGv2, we evaluated the effects of alternative methods for estimating plant C inputs. Keel et al. (2017) have pointed out the importance of the method of calculation of C inputs in modeling performance. We compared three methods for estimating aboveground plant C inputs (R, A1 and A2) and three methods for calculating belowground crop residues (B1–B3). In the reference method R (detailed in part 2.4.4), fixed HI values were used to calculate aboveground C inputs (C_{AG}) regardless of crop yields. In method A1, harvest index was calculated as a function of crop yield using coefficients from Fan et al. (2017) who found linear correlations between HI and crop yields and suggested that these relationships should improve estimations of crop residue inputs in cold continental climates. Method A2 was similar to A1, but used “local coefficients” for four major crops (wheat, winter barley, maize and pea) derived from French experimental data. The Bolinder approach was used for crop species which were not referenced by Fan et al. (2017). All coefficients are reported in Table S4.

Recent studies suggested that belowground inputs (C_{BG}) should be estimated regardless of crop yield or aboveground biomass using crop specific fixed values and/or dependent on farming systems (Taghizadeh-Toosi et al., 2016; Hirte et al., 2017; Hu et al., 2018). In the three methods B, aboveground inputs (C_{AG}) were calculated using the reference approach while BG input estimates (C_{BG}) were fixed for each crop species. In method B1, C_{BG} was calculated for each crop as the average of all C_{BG} estimates obtained for this crop in our database with the reference approach. Method B2 was similar but C_{BG} was decreased by 50% whereas it was increased by 50% in method B3, in order to

account for uncertainties on the shoot:root ratio estimates which show a coefficient of variation close to 50% (Bolinder et al., 2007). In all three methods, the belowground estimates included the dead root material (C_R) and the extra-root material (C_E), the latter being assumed to represent 65% of root material, as proposed by Bolinder et al. (2007). The potential mineralization rate k_0 was re-optimized for each method.

2.5.3. Assessment of the size of the stable C pool

Using AMGv2, we compared three methods (M1-M3) of parameterization of the initial stable pool fraction (C_S/C_0). In method M1, fixed values of C_S/C_0 were compared with those often recommended in other models as previously performed in Saffih-Hdadi and Mary (2008): we compared three values covering the range of usually reported values: 65%, 40% and 10% for soils with a long-term arable history. The proportion was reduced by 40% in soils with a long-term grassland history. For each parameter set, the potential mineralization rate k_0 was optimized giving three different k_0 values.

In method M2, we tested the hypothesis that C_S/C_0 is not constant but rather a decreasing function of SOC stock, suggesting that the active C pool could be proportionally higher in soils with high SOC content. We evaluated this hypothesis using the following empirical function:

$$\frac{C_S}{C_0} = P_S \cdot e^{-p \cdot QC_0} \quad (12)$$

where QC_0 is the initial SOC stock (t C ha^{-1}). The parameter p was set at one of three values (0.001, 0.005 and 0.010) and the parameter P_S (the proportion of C_S/C_0 for very low SOC stocks) was optimized each time, while k_0 was fixed at its default value.

In method M3, C_S/C_0 was optimized separately in each of the 20 sites, assuming that all treatments of the same site had a similar stable C pool, using each of the three values of parameter k_0 determined in method M1.

2.6. Model evaluation

2.6.1. Statistical criteria

Statistical measurements of agreement between observed SOC stock change rates and predictions made by the RF and AMG models were performed by calculating the mean difference (MD , simulated minus observed value), the modeling efficiency (EF), the index of agreement (dI), the root mean squared error ($RMSE$) and the relative root mean squared error ($RRMSE$) (Smith et al., 1996; Wallach, 2006; Willmott et al., 1985). The average values of MD and $RMSE$ obtained in each

experiment were used to calibrate the potential mineralization rate k_0 , which has to be optimized for each version of the model. A trial-and-error method was applied to determine the k_0 value that allowed to minimize both criteria. The same procedure was performed to determine the best values of parameters that were optimized when assessing the different C input calculation methods and when optimizing the C pool partitioning.

The predictive quality of AMGv1 and AMGv2 models was assessed by calculating the root mean squared error of prediction ($RMSEP$) using leave-one-out cross-validation (Stone, 1974). The evaluation was carried out each time on one site excluded from the calibration of k_0 , which was optimized using the data of the 19 remaining sites. The mean $RMSEP$ of the 20 situations was computed to compare the predictive quality of AMGv1 et AMGv2.

The coefficient of variation (CV) of measured SOC stocks was used to compare the measurement error with the relative model error ($RRMSE$).

2.6.2. Sensitivity analysis to input variables

We adapted the method conducted by Poeplau (2016) for the sensitivity analysis of RothC model. We analyzed the sensitivity of AMGv2 outputs to a 20% increase in several variables related to C inputs (crop yields, aboveground and belowground C inputs) and SOM mineralization (rainfall, PET, initial size of the active C pool, soil C:N ratio, clay and CaCO_3 contents), except for temperature and pH which were increased by 2°C and 1 unit, respectively. To this end, we simulated the SOC stock evolutions of reference scenarios for all 60 treatments over an extended period of 100 years. We calculated for each treatment the difference in SOC stocks at the end of the simulation (steady state) between a modified scenario (increase of a variable) and the reference one and analyzed the variations observed for the 60 treatments on model outputs.

3. Results

3.1. Drivers and prediction of SOC stock change rates

For the 60 treatments, measured SOC stock changes ranged from -24.0 to $+7.1 \text{ t C ha}^{-1}$ between the start and the end of experiments (Table 1). Annual SOC stock change rates varied from -1.01 to $+0.45 \text{ t C ha}^{-1} \text{ yr}^{-1}$; the median and mean rates were -0.08 and $-0.20 \text{ t C ha}^{-1} \text{ yr}^{-1}$, respectively. The linear regression made to calculate these rates is meaningful, since the $RMSE$ was small (1.2 t C

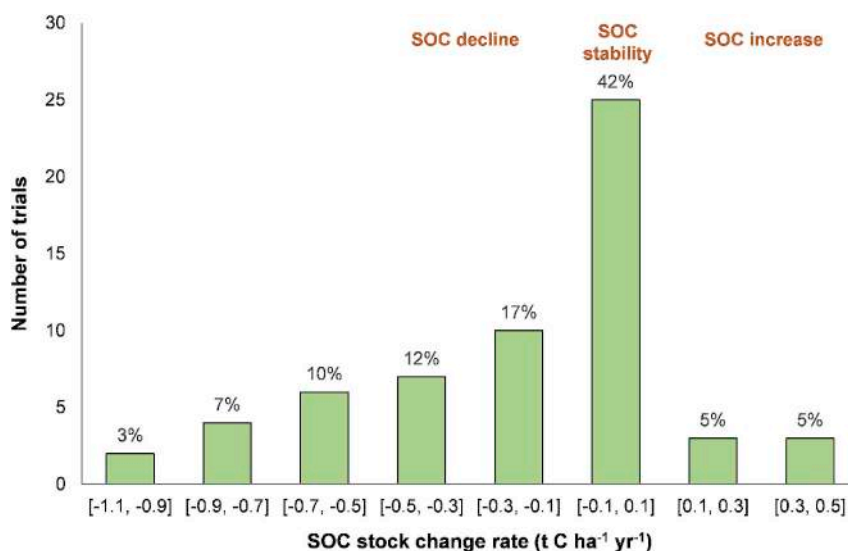


Fig. 2. Distribution histogram of SOC stock change rates over the 60 field trials.

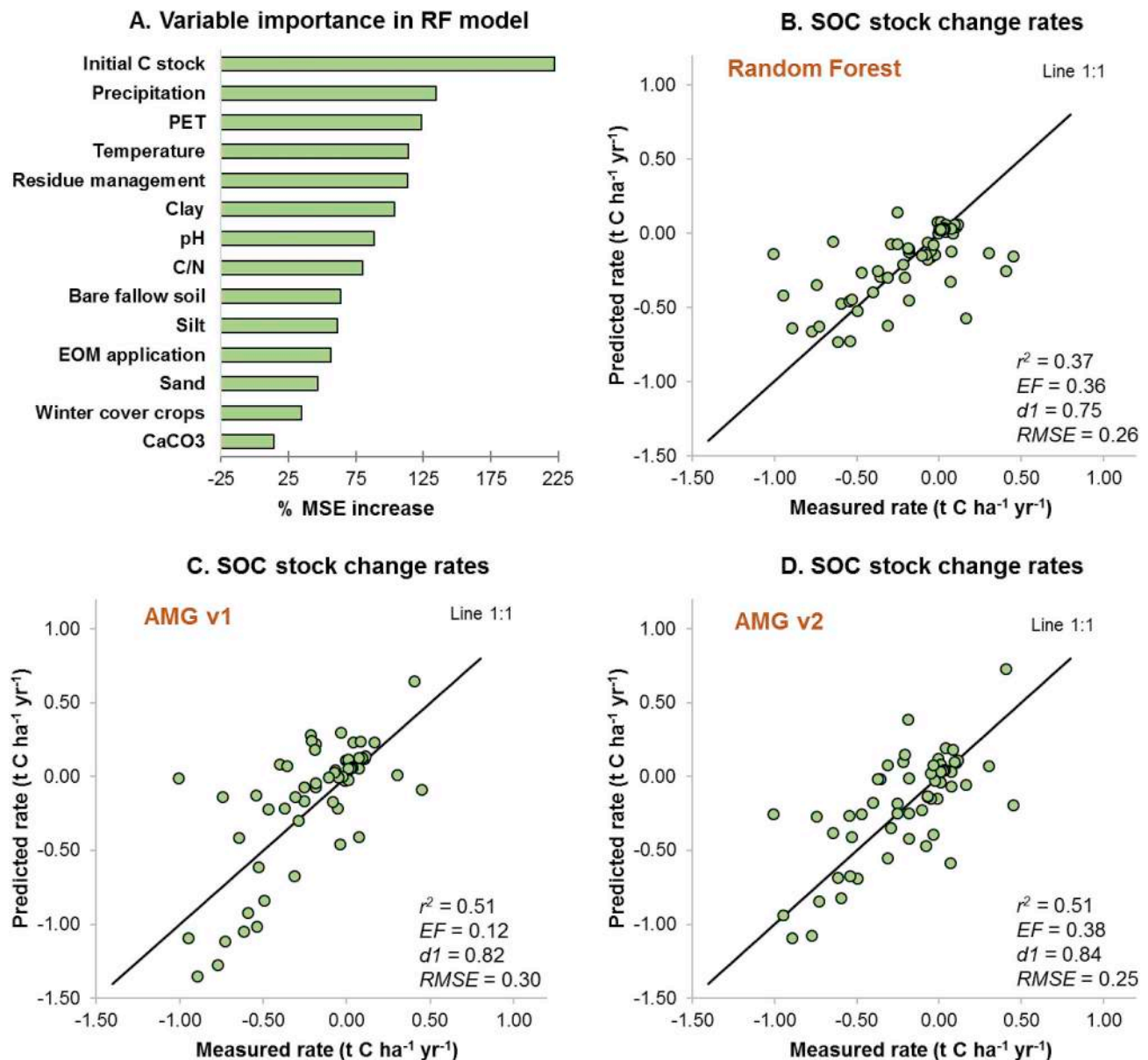


Fig. 3. Variable importance in a random forest (RF) model predicting SOC stock change rates for the 60 field trials (A) and observed vs predicted variations obtained with the Random Forest (B), AMGv1 (C) and AMGv2 (D) models. SOC: soil organic carbon, EF : modeling efficiency, $d1$: index of agreement, $RMSE$: root mean squared error of the model.

ha⁻¹) compared to the mean standard deviation of measurements (2.3 t C ha⁻¹), indicating that the general evolution of SOC was more or less linear over time. The distribution of SOC change rates was skewed towards negative values (Fig. 2). The interval [-0.1, 0.1] t C ha⁻¹ yr⁻¹ corresponds to the mean standard deviation of measurements and can be considered as a SOC stock stability range. It represented 42% of situations. SOC declined in 49% of situations and SOC increase occurred in the remaining 10% of situations.

The Random Forest (RF) analysis revealed that the initial C stock was the most important variable in predicting SOC stock change rate (Fig. 3A); indeed, the two variables are negatively correlated (Pearson $r = -0.59$, $p < 0.001$). The variables related to climate (precipitation, PET and temperature) were the second most important factor followed by the management of crop residues and soil parameters (clay, pH and C/N). The remaining input variables had less importance in the RF model applied on our dataset. Significant correlations were found between SOC stock change rate and precipitation ($r = -0.44$, $p < 0.001$) and PET ($r = 0.37$, $p < 0.01$) but no clear relationship was found with

the other variables.

Measured rates of SOC stock change were compared with predicted rates either by the RF model (Fig. 3B) or by simulations performed by AMG models: AMGv1 (Fig. 3C) and AMGv2 (Fig. 3D). The closeness of fit to the 1:1 line shows that there was no marked bias in the predictions made by the three models, MD varying between 0.00 and -0.05 t C ha⁻¹ yr⁻¹. The range of predicted rates was narrower for RF than for measured values. Overall, the statistical criteria revealed that AMGv2 performed better in predicting SOC stock change rates than RF and AMGv1 showing a higher modeling efficiency (EF) and index of agreement ($d1$), and a lower modeling error ($RMSE$).

3.2. Modeling SOC stock dynamics with AMG model

An example of SOC stock evolution and simulation performed by AMGv2 on one experiment at the Boigneville site is illustrated in Fig. 4. The model reproduced well the dynamics of total SOC stocks, accounting for the effects of straw residue export which led to a slight

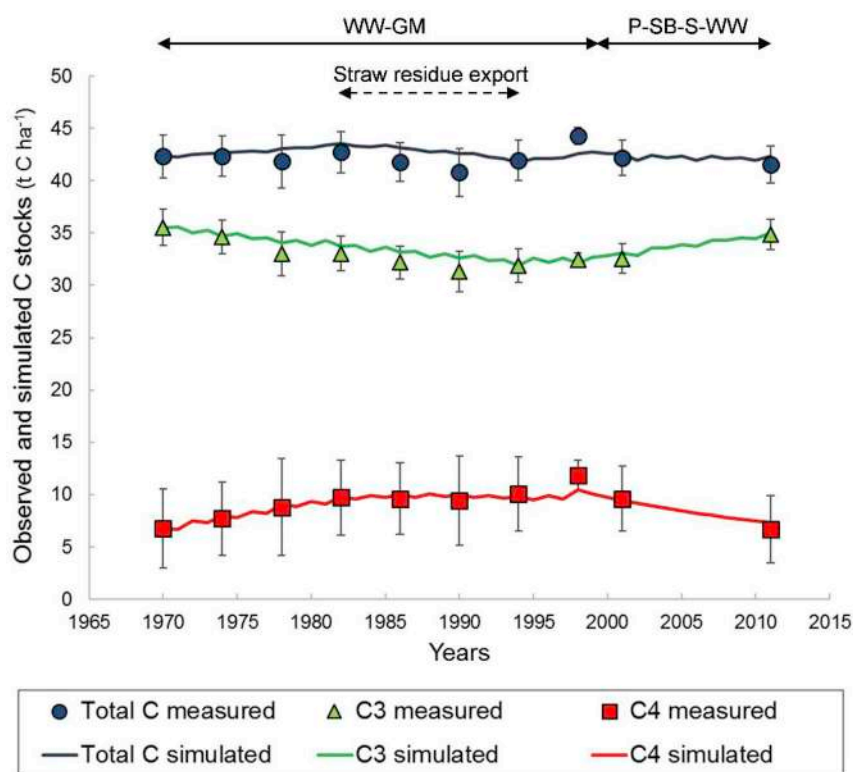


Fig. 4. Example of observations (symbols) and simulations performed by AMG (solid lines) of SOC stock evolutions in the upper soil layer (29 cm depth) of one treatment of the Boigneville long-term experiment (BOIG_A_CM4_L0). Circles represent total SOC stocks, while triangles and squares represent C stocks originating from C₃ and C₄ crops, respectively. Crop abbreviations: WW = Winter Wheat, GM = Grain Maize, P = Pea, SB = Spring Barley, S = Sugarbeet. Error bars are measured SD.

decrease in C stock between 1982 and 1994 and the change in crop rotation which occurred in 1998. It also simulated satisfactorily the evolution of C stocks originating from C₃ and C₄ crops, particularly the decrease in C₄ stock after changing the 2-year wheat-maize rotation to a 4-year rotation without C₄ crops.

The ability of AMGv1 and AMGv2 to predict SOC stock evolution was evaluated in the 60 field treatments (Fig. 5). Fig. 5A and B shows the absence of marked bias in the simulation of total SOC stock with both model versions. Fig. 5C and D shows that there was no increase in model error over time for the different C stocks simulated by both AMG versions. The mean modeling error was lower for AMGv2 than for AMGv1, *RMSE* being respectively 2.6 and 3.2 t C ha⁻¹ for total SOC stocks. The mean modeling error for C₃ stocks was also smaller for AMGv2 (*MD* = -0.5 and *RMSE* = 2.9 t C ha⁻¹) than for AMGv1 (*MD* = -1.1 and *RMSE* = 3.9 t C ha⁻¹). The predictive quality of AMGv2 was better than that of AMGv1, *RMSEP* being respectively 2.7 and 3.5 t C ha⁻¹ for total SOC stocks, when estimated using a cross-validation method. Compared to AMGv1, the modified version AMGv2, including the new mineralization function established on a completely independent dataset, was found to improve the prediction of SOC evolutions on long-term experiments.

AMGv2 was also tested on the database reported by Saffih-Hdadi and Mary (2008). We obtained a similar quality of fit than that found by these authors with the previous AMG version (mean *RMSE* of 1.6 t C ha⁻¹ for both versions). All results validated the reliability of this new version, which was therefore used in the following analyses.

3.3. Sensitivity analysis of AMGv2 model

The sensitivity analysis of AMGv2 was conducted on steady state situations. The reference scenario simulating the 60 treatments over a 100-year period predicted that the proportion of active pool C would reach an asymptotic value close to the initial value (35% of total C) for situations either with no export of straw biomass or with straw removal but receiving EOM applications (Fig. S1). The proportion of active C would, on average, stabilize around 20% of SOC for situations with

systematic straw residue removal.

The final SOC stocks simulated for this reference scenario were compared with those obtained in alternative scenarios in which one variable related to C input or SOM mineralization (depending on climate and soil properties) was increased. The mean SOC difference at steady state between the alternative and reference scenarios ranged from -4.1 to +2.7 t C ha⁻¹, depending on the input variable modified (Fig. 6). Variations in crop yield had a rather marked effect on SOC stocks (mean + 2.7 t C ha⁻¹), and corresponded to the sum of aboveground and belowground C effects. The model was particularly sensitive to changes in temperature, soil pH and C/N ratio, whereas changes in precipitation and PET affected very little the SOC stocks. The largest variability between sites in model response concerned soil pH. The initial size of the active C pool was also an important factor determining SOC stock at steady state. This emphasizes the importance of the variables with the largest uncertainty, *i.e.* plant C inputs calculated from crop yields and the initial SOC pool partitioning.

3.4. Impact of alternative methods for estimating plant C inputs

We evaluated the effect of alternative methods for estimating AG and BG plant C inputs on SOC modeling with AMGv2, compared to the reference R (Table 2). Method A1, which considered variable harvest indexes depending on crop yields, increased slightly model error for the simulation of soil C stocks, *RMSE* being of 2.6 vs 2.8 t C ha⁻¹ for R and A1 methods, respectively. Method A2, which used local coefficients for calculating harvest indexes, produced slightly better simulations (*RMSE* = 2.7 t C ha⁻¹) than A1 but did not improve SOC simulation compared to the reference. The alternative method of calculation of belowground inputs, in which root biomass was assumed to be only species dependent, did not affect much the quality of fit, as can be seen with method B1. However, when root biomass was reduced by 50% (method B2), SOC stock predictions were slightly improved for total SOC (*RMSE* = 2.5 t C ha⁻¹) and particularly for C₄ stocks for which the bias observed in the reference method disappeared. Conversely, a 50% increase in root C input (method B3) resulted in a poor quality of fit,

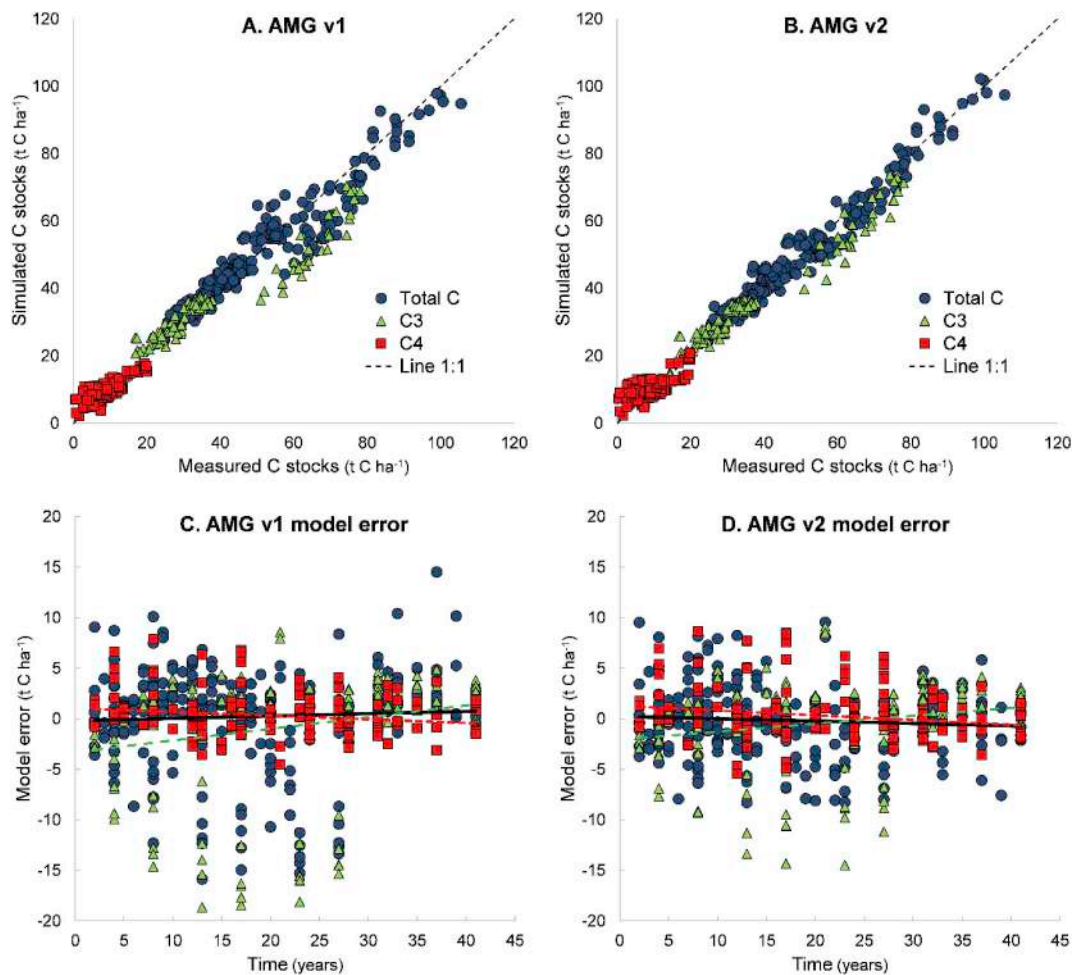


Fig. 5. Measured vs predicted SOC stocks by the AMGv1 (A) and AMGv2 (B) models and error (difference between simulated and measured SOC stocks) over time of AMGv1 (C) and AMGv2 (D) for all sampling dates of the 60 field-trials. Circles represent total SOC stocks, while triangles and squares represent C stocks originating from C3 and C4 crops, respectively. The solid line represents the regression line between model error and time for total C, while the red and green dotted lines represent the regressions for C originating from C4 and C3 crops, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

both for total SOC and C₄ stocks. It must be noticed that the reduction of root input in method B2 is accompanied by a reduction in the potential mineralization rate k_0 which drops from 0.29 to 0.24 yr⁻¹.

3.5. Impact of alternative methods for initializing the stable SOC pool

Three alternative methods (M1–M3) were assessed using AMGv2 for setting the size of the initial stable SOC pool (Table 3). Method M1 compares the effects of three values for the initial stable pool proportion (C_S/C_0). Results show that decreasing C_S/C_0 from the default value of 0.65 (for sites with long-term arable history) to 0.40 or 0.10 decreased the quality of fit for the simulations of total SOC, particularly for C₃ and C₄ stocks, increasing both the bias and the RMSE. The mineralization rates k_0 , optimized for each initial C_S/C_0 value (0.65, 0.40 and 0.10), dropped from 0.29 to 0.17 and 0.11 yr⁻¹, respectively.

In method M2, we tested the hypothesis that C_S/C_0 could be a decreasing (exponential) function of SOC stock. One parameter of this function (p) was fixed and the other (P_S) was optimized. This hypothesis proved to be inappropriate since model performance declined compared to the reference whatever the value of parameter p . The quality of fit decreased gradually as the slope of the exponential function increased.

In method M3, the size of the stable C pool was supposed to be site specific. The optimized mineralization rates k_0 obtained in method M1

were used as fixed parameters whereas C_S/C_0 was optimized for each site. This assumption resulted in a decreased model error for the simulations of total SOC stocks compared to the reference approach, whatever the k_0 value. The RMSE obtained with the default k_0 value of 0.29 yr⁻¹ was 1.8 t C ha⁻¹, lower than those obtained for k_0 values of 0.17 and 0.11 yr⁻¹ (RMSE = 2.0 and 2.4 t C ha⁻¹, respectively). In addition, these alternative k_0 values (corresponding to low values of C_S/C_0) did not allow to simulate C₃ and C₄ stocks and generated an important bias on each stock (up to 3.5 t C ha⁻¹). The variability of C_S/C_0 values optimized on each site for each k_0 value is shown in Fig. 7. The median C_S/C_0 values obtained for the 20 sites (0.63, 0.37 and 0.08) were close to the single values initially applied to all sites (0.65, 0.40 and 0.10). The variability of C_S/C_0 between sites was much lower for the default value of k_0 (0.29 yr⁻¹) than for the two other settings.

4. Discussion

4.1. Observed SOC evolution in arable cropping systems

The dataset considered in this study covers a period ranging from 1970 to 2015, the average being a 24-year period (1980–2003). It covers the diversity of arable cropping systems practiced in France during these years, with regard to crop rotations, tillage practices, crop residue management, N fertilization and crop yields. During the more

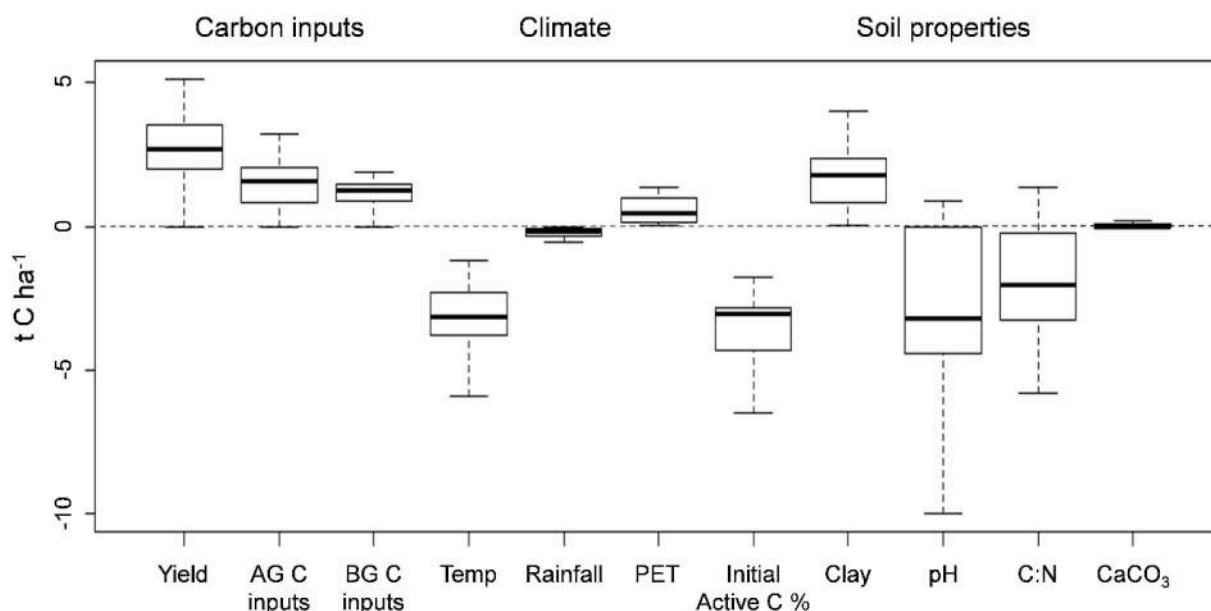


Fig. 6. Boxplots showing the sensitivity of the AMGv2 model to 20% increase in different variables/parameters related to C inputs and SOM mineralization, excepting temperature and pH which were increased by 2 °C and 1 pH unit, respectively. Boxplots represent the variations of the differences between the modified scenario (increase of the variable) and the reference scenario for all 60 trials over an extended period of 100 years. The dotted line represents the result for the simulation of final SOC stocks in the reference scenario with unmodified data and parameters. Boxplots show median and quartiles, while whiskers represent samples lying within 1.5 times the interquartile range. Extreme outliers are not shown.

recent years, an evolution towards a higher frequency of catch crop cultivation and a slight reduction in tillage operations and intensity was observed. Our results showed on average a slight decrease in SOC stocks (mean rate of change = $-0.20 \text{ t C ha}^{-1} \text{ yr}^{-1}$). This decrease could be attributed to the legacy effect of conversion from grass to arable land over the past 25 years with comparatively lower organic matter restitution levels. In many regions, the areas devoted to permanent meadows have declined regularly as exemplified in the Seine-Normandie Basin between 1971 and 2013 in North of France (Beaudoin et al., 2018). Steinmann et al. (2016) observed a drastic decline under arable crops in Germany between 1989 and 2015, which was also mainly attributed to grassland conversion to cropland. This is consistent with other results obtained on conventional arable systems under temperate climate. For example, Saffih-Hdadi and Mary (2007) gathered a set of 391 agricultural fields monitored several times in Picardie (Northern France) during the 1970–1997 period and found a mean decrease rate of $-0.08 \text{ t C ha}^{-1} \text{ yr}^{-1}$. In Belgium, Goidts and van Wesemael (2007) reported a decrease of $-0.11 \text{ t C ha}^{-1} \text{ yr}^{-1}$ in arable crops during 50 years (1955–2005) confirmed by Meersmans et al. (2011) who observed a mean decrease of $-0.09 \text{ t C ha}^{-1} \text{ yr}^{-1}$ from 1960 to 2006.

4.2. Drivers of SOC dynamics

The main drivers of SOC dynamics identified by RF were the soil characteristics (initial SOC stock, texture, ...), the agricultural practices (residue management, cover crops, EOM) and the climate (precipitation, temperature). The initial SOC stock was a main factor as shown by the RF analysis and the negative correlation between SOC change rates and the initial SOC stock. Such a strong negative relationship was already pointed out by Goidts and van Wesemael (2007), Zhao et al. (2013) and Luo et al. (2017). It suggests that soils with the highest SOC contents, with past grassland or having received important amounts of EOM, were not yet at equilibrium and are still declining. This is consistent with Oberholzer et al. (2014) who found that SOC content was still declining even 60 years after the conversion of grassland to cropland. Post et al. (2008) have pointed out the importance of an accurate determination of initial SOC stock in the propagation of uncertainty in

SOM models.

Residue management (straw removal vs retention) was also an important factor identified by both RF and AMG model. This confirms the results obtained by Saffih and Mary (2008) and Liu et al. (2014). Reducing residue removal increased SOC in most wheat cropping systems studied in Australia by Zhao et al. (2013) and Luo et al. (2017).

The impact of climatic factors was more surprising: the temperature effect was consistent between RF analysis and AMG model, but not precipitation, which was an influent factor in RF but not in AMG. This apparent contradiction is due to the fact that precipitation was strongly correlated with initial SOC content ($r = 0.59$, $p < 0.001$). In fact, running the RF analysis without this variable explained as much variance than with it. The small sensitivity of AMG model reflects the moderate range of water balance (P-PET varied from -290 to 595 mm yr^{-1}) in all sites, without dry situations such as described by Luo et al. (2017). Indeed, we confirmed the absence of improvement in model performance when recalibrating this function. Taghizadeh-Toosi et al. (2014) also found that there was no need to account for moisture effects in the C-TOOL model to simulate the data obtained in three LTEs of Northern Europe.

Finally, two other soil characteristics were identified as being influent on SOC evolution: the C/N ratio and soil pH. Both were identified in this study by the Random Forest analysis and previously as drivers of organic N mineralization (for more discussion see Clivot et al., 2017), justifying the implementation of these variables and their effect in AMGv2.

The model could simulate the LTEs without considering nitrogen (N) availability as a possible driver of SOC evolution, as suggested by the C:N stoichiometry observed in SOM composition (van Groenigen et al., 2017). This may result from the positive N surplus observed in most of our experiments, but a possible limitation should be considered in other experiments, particularly those receiving low N inputs.

4.3. Reliability of AMG model

The new AMG version was found to better predict SOC stock change rates than RF and AMGv1. The general evolution of SOC was found to

Table 2
Evaluation of the quality of fit obtained with AMGv2 using different methods for estimating aboveground and belowground C inputs.

Method for estimating C inputs	Harvest Index	Aboveground C inputs	Belowground C inputs	Optimized k0 value	Total SOC*			SOC-C3**			SOC-C4**		
					MD	RMSE	t C ha ⁻¹	MD	RMSE	t C ha ⁻¹	MD	RMSE	t C ha ⁻¹
R. Reference method (Bolinder et al., 2007)	HI = f(species)	C _{AG} = f(species, Y, HI)	C _{BG} = f(species, Y, HI, SR)	0.29	-0.1	2.6	-0.5	2.9	0.4	2.0	2.0		
A1. HI function of yield (Fan et al., 2017)	HI = f(species, Y)	C _{AG} = f(species, Y, HI)	C _{BG} = f(species, Y, HI, SR)	0.32	-0.1	2.8	-0.6	3.1	0.7	1.9	1.9		
A2. HI function of yield (local coefficients)	HI = f(species, Y)	C _{AG} = f(species, Y, HI)	C _{BG} = f(species, Y, HI, SR)	0.30	0.0	2.7	-0.5	3.0	0.6	1.9	1.9		
B1. Fixed root biomass	HI = f(species)	C _{AG} = f(species, Y, HI)	C _{BG} = f(species)	0.29	0.0	2.6	-0.4	2.9	0.5	2.0	2.0		
B2. Fixed root biomass - 50%	HI = f(species)	C _{AG} = f(species, Y, HI)	C _{BG} = 0.5* f(species)	0.24	-0.1	2.5	-0.3	2.7	0.0	2.0	2.0		
B3. Fixed root biomass + 50%	HI = f(species)	C _{AG} = f(species, Y, HI)	C _{BG} = 1.5* f(species)	0.34	0.0	2.8	-0.6	3.1	0.9	2.2	2.2		

Y = crop yield; HI = harvest index; SR = shoot:root ratio.
 * whole database (60 field trials).
 ** subset (27 field trials).

be more or less linear over time. However, on the contrary to AMG, RF is a statistical model which cannot capture subtle changes in SOC through time since RF, as used in this study, cannot take into account annual variations of climate and C inputs. In AMGv2, the implementation of two additional variables (soil pH and C/N ratio), previously identified as drivers of SOM mineralization (Clivot et al., 2017) but not considered in AMGv1, slightly improved the quality of SOC predictions, since the relative root mean square error (RRMSE) decreased from 6.1% for AMGv1 to 5.3% for AMGv2. This result was obtained with a common set of parameters for all sites, without any site-specific calibration. This model error was only slightly greater than the mean coefficient of variation of measurements which was 4.3%. Furthermore, the model error did not increase with time, showing that there was no significant drift over time. The model error is comparable to that obtained on other LTEs with other models. Smith et al. (1997) compared nine models on 7 LTEs and found a RRMSE varying between 6.5% and 10% for the best 6 models. Falloon and Smith (2002) simulated 6 LTEs and obtained a mean RRMSE of 6.8% for Century and 9.9% for RothC. The CCB model (Franko et al., 2011), evaluated on 40 sites in central Europe, showed a mean RRMSE of 8.5%. Taghizadeh-Toosi et al. (2014) evaluated the C-TOOL model on 3 LTEs in Northern Europe and obtained a mean RRMSE of 6.1% for topsoils. Using the Century model, Dimassi et al. (2018) obtained a RRMSE of 13.1% on a subset of our database with 6 LTEs.

Datasets including ¹³C natural tracing experiments (with C₄ and C₃ plants) are essential to better evaluate SOM models, because they allow to characterize separately the decrease in «old» SOM and the increase in newly formed SOM (Balesdent, 1996). The AMG model was shown to simulate well the evolution of C₃ and C₄ stocks in the experiments which included C₄ plants, showing its ability to simulate the two components of SOC change.

4.4. Uncertainties in plant C input estimates

C input estimates in our study are close to those obtained in comparable climatic conditions, reported by Wiesmeier et al. (2014) in Germany for cereals (3.2 vs 3.1 t C ha⁻¹ yr⁻¹) and for other crops (2.7 vs 2.3 t C ha⁻¹ yr⁻¹). These inputs, which represent annually 5.3% of SOC on average, include uncertainties on aboveground inputs, particularly on the harvest index. The model performance was little sensitive to the method of calculation: the model did not perform better when using a variable HI calibrated with French references compared to the original Bolinder method with a fixed HI. Comparing five different methods, Keel et al. (2017) also found that the Bolinder method gave the best predictions of SOC evolution using the C-TOOL model. However, the greatest uncertainties about C input are those relating to belowground C. For root biomass estimates, we found little difference in model performance when using allometric equations (R) or fixed biomass (B1). Taghizadeh-Toosi et al. (2016) made the same comparison with the C-TOOL model and obtained a better quality of fit when using the fixed root biomass option. Recent studies suggest that root biomass could be independent of aerial biomass, questioning the rationale of allometric relationships. Hirte et al. (2018) found that N fertilization rate affects the below:above ground ratio of wheat and maize but does not modify the belowground C inputs. Komainda et al. (2018) found no effect of N fertilization on root biomass and turnover in two cultivars of maize. Hu et al. (2018) even found larger root biomass of cereals and catch crops in organic farming than in conventional systems, in spite of a lower aerial biomass. Therefore, using a fixed amount of root biomass depending on crop species only seems to be a preferable option for simulating SOC evolution.

Concerning the BG inputs, our results show that model performance (including the prediction of C₄ stocks) markedly declined when increasing BG inputs beyond the default fixed root biomass (method B1). This indicates that the contribution of root and extra root material (65% of root material, i.e. 40% of BG inputs) to the humified C input is set at

Table 3
Evaluation of the quality of fit obtained with AMGv2 using three methods and three parameterizations for setting the size of the initial stable pool proportion (C_S/C_O).

Method	Initial stable pool fraction (C_S/C_O)	Fixed parameter	Fixed parameter	Optimized parameter	Total SOC		SOC-C3		SOC-C4		
					MD	RMSE	MD	RMSE	MD	RMSE	
					t C ha ⁻¹	t C ha ⁻¹	t C ha ⁻¹	t C ha ⁻¹	t C ha ⁻¹	t C ha ⁻¹	
M1	Constant	Fixed		C_S/C_O 0.65 *	k_O 0.290	-0.1	2.6	-0.5	2.9	0.4	2.0
		Fixed		C_S/C_O 0.40 *	k_O 0.170	0.0	2.9	-1.5	2.3	2.3	2.9
		Fixed		C_S/C_O 0.10 *	k_O 0.115	-0.1	3.3	-2.5	3.2	3.5	4.2
M2	Variable	$C_S/C_O = P_s \cdot \exp(-p \cdot QC_O)$	k_O 0.290	p 0.001	P_s 0.66	0.0	2.9	0.6	2.1	0.4	2.0
		$C_S/C_O = P_s \cdot \exp(-p \cdot QC_O)$	k_O 0.290	p 0.005	P_s 0.83	-0.1	3.4	1.0	2.5	0.4	2.0
		$C_S/C_O = P_s \cdot \exp(-p \cdot QC_O)$	k_O 0.290	p 0.010	P_s 1.00	-1.3	4.1	0.1	2.9	0.4	2.0
M3	Site specific	Fixed	k_O 0.290		C_S/C_O Site specific **	0.1	1.8	-0.4	2.3	0.4	2.0
		Fixed	k_O 0.170		C_S/C_O Site specific **	0.1	2.0	-2.3	2.9	2.3	2.9
		Fixed	k_O 0.115		C_S/C_O Site specific **	0.7	2.4	-2.6	3.3	3.5	4.2

* Values reduced by 40% in the site with long term grassland history.
** The variabilities of C_S/C_O values optimized for the 20 sites are shown in Fig. 7.
Line in bold corresponds to the reference method.

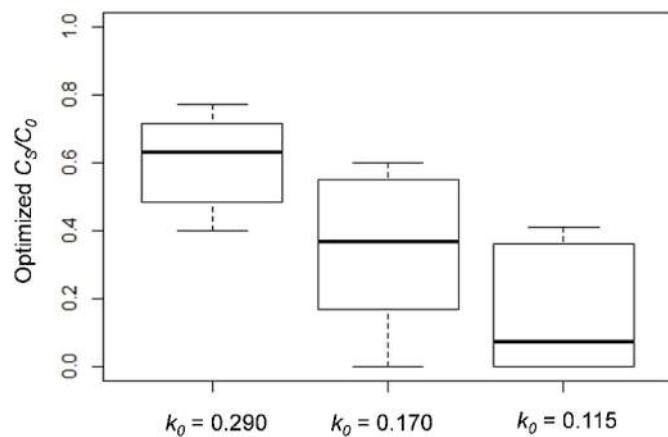


Fig. 7. Variability of the initial stable C pool proportion (C_S/C_O) optimized for each site ($n = 20$) for three different values of the potential mineralization rate (k_0). Boxplots show median and quartiles, while whiskers represent samples lying within 1.5 times the interquartile range. Extreme outliers are not shown.

its maximum and could even be overestimated. A similar conclusion on extra root C was drawn by Poehlau (2016) with the RothC model, while results from a recent field study (Hirte et al., 2018) suggest that the proportion of rhizodeposition of total BG inputs for maize and wheat should be higher (on average 55% in the topsoil for net rhizodeposition C) than the widely adopted value of 40%. However, besides the uncertainty on the amount of extra root material deposited, it should be noticed that the humification coefficient applied to this fraction in our model is equivalent to that of roots, whereas root exudates are very labile substances and might contribute less to SOC formation.

4.5. Initializing the size of the stable SOC pool

The sensitivity analysis indicated that the initial setting of the inert SOC pool had a large impact on model outputs, confirming previous studies (e.g. Puhlmann et al., 2007). The site-specific adjustment of SOC pools gave better simulations than default parameterization, since the RRMSE reduced from 5.3 to 3.7% as previously observed with Century and RothC models (Falloon and Smith, 2002). However, the lack of

information on the past land use (particularly the grassland history) did not allow us to calculate a more precise initial partitioning of SOC between pools.

During the calibration phase, the optimization of the size of the recalcitrant C pool (either inert or having a residence time greater than 1000 years) is highly dependent on the value of the potential rate constant of the active C pool, because both are correlated. The strong correlation between the two parameters may even result in equifinality, i.e. leading to similar model performance for widely varying paired parameter values (Luo et al., 2016). This was not the case with our dataset and model, since the model error increased significantly, particularly for the C_4 stocks simulations, when the initial stable pool fraction was reduced from 65% to 10%. The mean value found in optimizing the site-specific C_S/C_O was $60 \pm 18\%$ for sites with a long-term arable history and was found to be lower (i.e. 47%) for the site with long-term grassland history. This result confirms the default parameterization established earlier (Saffih-Hdadi and Mary, 2008).

Chemical methods have been proposed to characterize the more stable SOC fractions with a limited success (Helfrich et al., 2007; von Lützw et al., 2007). Combining particle size fractionation and chemical analysis was more successful in separating SOC into fractions with different turnover rates (Poehlau et al., 2018) and in matching measurable C fractions and model pools (Zimmermann et al., 2007; Herbst et al., 2018). New methods such as thermal analysis are also promising: they could allow identifying fractions having a residence time of about 20 years (Soucémariadin et al., 2018), these latter corresponding to the residence time in our experiments (varying from 7 to 26 years). Data from long-term bare fallow experiments (Barré et al., 2010) can also be combined with thermal analysis to quantify the size of centennially persistent SOC pool (Cécillon et al., 2018) in order to better calibrate soil C models.

5. Conclusion

The modified version of AMG model including the new function of SOM mineralization was found to improve the prediction of SOC evolution compared to the previous version. The model could simulate SOC stock dynamics in LTEs conducted in French conventional arable systems with a mean relative model error of 5.3%. The results strengthen the importance of SOC pool partitioning and therefore the need of

methods that would allow to measure functional C fractions to better initialize soil C model simulations. The model performance appeared to be little sensitive to the method of plant C input estimation. Considering root C inputs independent of aerial biomass production as shown by recent studies was found to perform as well as allometric relationships, suggesting that using a fixed amount of root biomass depending on crop species should be preferred in the model. AMG demonstrates a good potential for predicting SOC evolution in scenarios varying in climate, soil properties and management for conventional arable cropping systems. The next objective will be to improve the ability of AMG for modeling other systems such as low input or organic systems, cropping systems including perennial species or permanent grasslands in order to extend the validity domain of the model to simulate contrasting agricultural systems.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.envsoft.2019.04.004>.

Appendix A. Model description and environmental functions and parameters used in AMGv1 and AMGv2 models

A.1. Model description

AMG is a model designed to simulate soil C dynamics at an annual time step (Andriulo et al., 1999; Saffih-Hdadi and Mary, 2008). The model considers three organic matter (OM) compartments: fresh OM (FOM) coming from crop residues or organic amendments which can be decomposed or humified, and SOM which is divided into active (QC_A) and stable C pools (QC_S).

AMG can be described by this set of equations:

$$QC = QC_S + QC_A \quad (2)$$

$$\frac{dQC_A}{dt} = \sum_i m_i h_i - kQC_A \quad (3)$$

where QC is the total SOC stock ($t\ ha^{-1}$), QC_A and QC_S are the C stocks of the active and stable C pools ($t\ ha^{-1}$) respectively, m_i is the annual C input from organic residue i ($t\ ha^{-1}\ yr^{-1}$), h is its humification coefficient and k is the mineralization rate constant of the active C pool (yr^{-1}).

The model allows simulating separately the C originating from C_3 or C_4 crops using ^{13}C natural isotopic abundance measurements. The C stocks originating from C_3 (QC_3) and C_4 (QC_4) crops were calculated using the following equations (Balesdent et al., 1987):

$$QC_3 = \frac{\delta^{13}C_S - \delta^{13}C_4}{\delta^{13}C_3 - \delta^{13}C_4} \cdot QC \quad (S1)$$

$$QC_4 = \frac{\delta^{13}C_S - \delta^{13}C_3}{\delta^{13}C_4 - \delta^{13}C_3} \cdot QC \quad (S2)$$

where $\delta^{13}C_S$ is the measured ^{13}C isotopic composition in the soil and $\delta^{13}C_3$ and $\delta^{13}C_4$ are the isotopic compositions of C_3 and C_4 crops in the rotation, respectively. The isotopic signatures defined in the model parameters for C_3 and C_4 residues are directly applied to their humified fractions. The isotopic signatures of C_3 and C_4 humified plant residues were set by default at -27.5% and -12.5% of $\delta^{13}C$, respectively. These values are close to those reported for C_3 and C_4 plants and we assume that $\delta^{13}C$ of SOM is about equal to that of plant materials from which it is derived (Balesdent et al., 1987). The proportion of QC_4 being part of the stable C compartment at the start of the experiment (PC_{4S}) can be specified in the model or optimized to define the distribution of C originating from C_4 crops between the active (QC_{4A}) and stable pools (QC_{4S}):

$$QC_{4S} = PC_{4S} \cdot QC_4 \quad (S3)$$

$$QC_{4A} = QC_4 - QC_{4S} \quad (S4)$$

The partitioning of C originating from C_3 crops between the active (QC_{3A}) and stable pools (QC_{3S}) was therefore calculated as follows:

$$QC_{3A} = QC_A - QC_{4A} \quad (S5)$$

$$QC_{3S} = QC_S - QC_{4S} \quad (S6)$$

A.2. Environmental functions and parameters

In AMGv1 and AMGv2, the mineralization rate k of the active C pool is calculated using environmental functions following these equations:

$$k_{AMGv1} = k_0 \cdot f(T) \cdot f(H) \cdot f(A) \cdot f(CaCO_3) \quad (4)$$

$$k_{AMGv2} = k_0 \cdot f(T) \cdot f(H) \cdot f(A) \cdot f(CaCO_3) \cdot f(pH) \cdot f(C/N) \quad (5)$$

where k_0 is the potential mineralization rate (in yr^{-1}) set at 0.165 and 0.290 for AMGv1 and AMGv2, respectively.

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In both AMG versions, $f(T)$ is a function of mean annual air temperature T (°C):

$$f(T) = \frac{a_T}{1 + b_T \cdot \exp(-c_T \cdot T)} \quad (S7)$$

with $f(T) = 0$ if $T \leq 0$

$$\text{and } b_T = (a_T - 1) \cdot \exp(c_T \cdot T_{Ref}) \quad (S8)$$

with $a_T = 25$, $c_T = 0.120 \text{ K}^{-1}$ and $T_{Ref} = 15$ °C.

$f(H)$ is a function used as a proxy to describe the effects of soil moisture. These effects are calculated in $f(H)$ as a function of the difference between cumulative annual water inputs (precipitation P and irrigation water IW) and potential evapotranspiration PET (in mm):

$$f(H) = \frac{1}{1 + a_H \cdot \exp\left(-b_H \cdot \frac{P - PET + IW}{1000}\right)} \quad (S9)$$

with $a_H = 3.0 \cdot 10^{-2}$ and $b_H = 5.247 \text{ m}^{-1}$

Function $f(A)$ and $f(\text{CaCO}_3)$ are describing the effects of clay (A) and CaCO_3 (CaCO_3) contents (g kg^{-1}) on SOM mineralization, respectively:

$$f(A) = \exp(-a_m \cdot A) \quad (S10)$$

with $a_m = 2.720 \cdot 10^{-3}$ and $2.519 \cdot 10^{-3}$ (g kg^{-1}) in AMGv1 and AMGv2, respectively.

$$f(\text{CaCO}_3) = \frac{1}{1 + c_m \cdot \text{CaCO}_3} \quad (S11)$$

with $c_m = 1.67 \cdot 10^{-3}$ and $1.50 \cdot 10^{-3}$ (g kg^{-1}) in AMGv1 and AMGv2, respectively.

In AMGv2, the additional functions $f(pH)$ and $f(C/N)$ are describing the effects of soil pH and C/N ratio on SOM mineralization:

$$f(pH) = \exp(-a_{pH} \cdot (pH - b_{pH})^2) \quad (S12)$$

with $a_{pH} = 0.112$ and $b_{pH} = 8.5$

$$f(C/N) = 0.8 \cdot \exp(-a_{CN} \cdot (C/N - b_{CN})^2) + 0.2 \quad (S13)$$

with $a_{CN} = 0.060$ and $b_{CN} = 11$.

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