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Rock-Eval® Thermal Analysis Meets Machine Learning for Accurate Initialization of a Soil Carbon Model

Marija Stojanova[1,2], Fabien Ferchaud[3,4], Hugues Clivot[5], Lauric Cécillon[6], Adrian Andriulo[7], François Baudin[8], Claire Chenu[9], Bent T. Christensen[10], Kenji Fujisaki[11], Thomas Kätterer[12], Florent Levavasseur[9], Ines Merbach[13], Christopher Poeplau[14], Jonathan Sanderman[15], Pierre Barré[1]

Correspondence to: Pierre Barré (barre@geologie.ens.fr)

[1]Laboratoire de Géologie, École Normale Supérieure, CNRS, PSL University, IPSL, Paris, France.
[2]ENS de Lyon, LGL-TPE, UMR 5276, Université Claude Bernard Lyon1, UJM Saint-Etienne, CNRS, Lyon, France
[3]UMR Eco&Sols, Univ Montpellier, CIRAD, INRAE, IRD, Institut Agro, Montpellier, France.
[4]BioEcoAgro Joint Research Unit, INRAE, Université de Liège, Université de Lille, Université de Picardie Jules Verne, 02000, Barenton-Bugny, France
[5]Université de Reims Champagne-Ardenne, INRAE, FARE, UMR A 614, Reims, France
[6]Ministère de l'Europe et des affaires étrangères, Ambassade de France au Kénya, Nairobi, Kenya
[7]INTA, Pergamino, Buenos Aires, Argentina
[8]Sorbonne Université, CY Univ., CNRS, ISTeP, 75005, Paris, France
[9]Université Paris-Saclay, INRAE, AgroParisTech, UMR ECOSYS, 91120, Palaiseau, France
[10]Department of Agroecology, Aarhus University, Tjele, Denmark
[11]INRAE, Info&Sols, 45075, Orléans, France
[12]Department of Ecology, Swedish University of Agricultural Sciences, Uppsala, Sweden
[13]Department of Community Ecology, Helmholtz Centre for Environmental Research-UFZ, D-06120, Halle, Germany
[14]Thünen Institute of Climate-Smart Agriculture, Braunschweig, Germany
[15]Woodwell Climate Research Center, Falmouth, Massachusetts, USA

Abstract. In recent years, a growing number of policies related to soil organic carbon (SOC) have been developed, creating an urgent need for tools capable of simulating and predicting changes in SOC stocks. Models dividing SOC into different kinetic pools are frequently used to estimate changes in SOC stocks. Accurate and robust initialization of these pools' sizes is a recurring obstacle for generating reliable simulations, calling into question their use as an actionable basis for these policies. In this study, we used an exceptional set of data including time series from 25 temperate long-term field experiments around the world to demonstrate that thermal stability and elemental stoichiometric composition of organic matter, as determined by Rock-Eval® thermal analysis, correlate with biogeochemical stability and that it is possible to use this information to initialize a compartmental model of SOC dynamics. First, we capitalized on the relative simplicity of the AMG model to optimize the initial allocation of carbon (C) between two kinetic pools (stable C and active C), resulting in the best fit between observations and AMG simulations. Second, we ensured that some SOC characterization results obtained using Rock-Eval® thermal

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analyses were correlated to the proportion of stable SOC sensu AMG. Third, we developed a data-driven support vector machine (SVM) model to estimate the proportion of stable SOC sensu AMG using only Rock-Eval® parameters. Fourth, we demonstrated that implementing our initialization method in AMG produced more accurate simulations compared to the default initialization. We argue that future adaptations of this approach can be used to initialize other compartmental models of similar complexity. Thus, our study represents a major game changer in the initialization of compartmental models, which are needed in the rapidly developing monitoring, reporting, and verification (MRV) sector.

1 Introduction

Soils constitute the largest terrestrial carbon (C) reservoir, with a stock of 2400 Pg in the upper two meters (Jobbagy and Jackson, 2000). Over the last 8000 years, agricultural soils have significantly contributed to climate change by releasing more than 100 Pg C to the atmosphere (Sanderman et al., 2017). In recent decades, several studies have shown that by applying appropriate farming practices, it is possible to restitute a part of this soil organic carbon (SOC) stock and thus contribute to climate change mitigation (Smith et al., 2008; Smith, 2016; Chenu et al., 2019; Petersson et al., 2025). The potential contribution of C accrual in agricultural soils has been estimated at 3-4 Gt CO2-eq year−1 in the latest IPCC report (2023), making it one of the main mitigation options available by 2030. In addition, the increase of SOC stocks also improves soil health and crop yields (Kätterer and Bolinder, 2024), which gives this no-regret, nature-based solution significant co-benefits (Kopittke et al., 2022).

In recent years, the issue of increasing SOC stocks has become a political priority (e.g., Vermeulen et al., 2019; FAO, 2019; Chenu et al. 2026). Countries that have signed the Paris Agreement can now include SOC storage in their nationally determined contributions (NDCs) to meet their climate mitigation commitments, and EU member states are under increasing pressure to assess and report their carbon sequestration potential, including that of agricultural soils, in the context of the European Climate Law (EU 2021). In addition, SOC sequestration in agricultural soils has also become an economic sector with the development of schemes that reward farmers implementing practices increasing SOC stocks (Paul et al., 2023). Most often, these schemes involve the use of models to quantify the expected SOC stocks changes in absolute terms or relative to the baseline SOC stock evolution under a reference, business-as-usual scenario (Dupla et al., 2024 ; Ihasusta et al., 2026).

However, recent studies have highlighted several limitations of currently-used models simulating SOC stock evolution in agricultural soils. Due to the limited availability of independent time-series data, models simulating SOC stock dynamics remain insufficiently validated (Le Noë et al., 2023; Garsia et al., 2023). Furthermore, these models most often divide SOC into different conceptual kinetic pools that do not correspond to measurable physical, chemical, or biological soil fractions. As a result, initializing the size of these pools at the beginning of the simulated period is a recognized problem that can strongly influence the simulated SOC stocks evolution (Luo et al., 2015; Laub et al., 2020, Ihasusta et al., 2027).

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A classic approach for SOC kinetic pools initialization is the spin-up method consisting of iteratively running the model until a SOC steady state is reached, such that it matches the initial SOC stock measurement of the simulated period (Wutzler and Reichstein, 2007; Taghizadeh-Toosi et al., 2020). The spin-up method, however, requires extensive data on climate, C inputs, land-use, and land cover for the years preceding the simulated period. When collected over a large time span, these data are often unreliable and prone to noise. Moreover, it is questionable whether a steady-state equilibrium can be seen as a justified choice at the onset of the simulation.

Some studies have proposed linking physical SOC fractionation or Mid-IR spectroscopy results to the size of kinetic pools as an alternative to the spin-up approach (e.g., Zimmermann et al., 2007; Skjemstad et al., 2004; Laub et al., 2020, 2024; Dangal et al., 2021). However, these methods have not been independently validated, or only to a very limited extent. More recently, Cécillon et al. (2018; 2021) developed a machine-learning model that quantifies the proportion of centennially-stable SOC using Rock-Eval® (RE) thermal analysis and its established correlation with biogeochemical stability (Barré et al., 2016). This model, named PARTYsoc v2.0, was trained on SOC biogeochemical stability data observed in long-term agricultural experiments (LTEs). Kanari et al. (2022) later used PARTYsoc v2.0 to successfully initialize the two kinetic pools (active and stable SOC) of the AMG v2.0 model (Clivot et al., 2019) for simulating changes in SOC stocks in mainland France agricultural soils. However, PARTYsoc v2.0 was trained using only sites whose centennially stable SOC fraction could be estimated: six long-term bare fallow (LTBF) sites in Europe and one vegetation change site in South America, potentially limiting its generalizability.

Given the urgent need for scientifically validated, actionable tools that can be used to support SOC-related policies, we have capitalized on these promising results to develop a new version of the PARTYsoc model specifically interfaced with the AMG model. We used an unprecedented dataset consisting of 25 worldwide temperate long-term field experiments having ready-to-use AMG data (Fujisaki et al., 2026), as well as Rock-Eval® thermal analysis data acquired on archive soil samples from these sites. Using an AMG-optimized stable SOC stock, we calculated a sample-wise stable SOC proportion. We first established robust correlations between soil organic matter (SOM) characteristics determined by Rock-Eval® thermal analysis, i.e. thermal stability and elemental stoichiometric composition, and AMG-optimized stable SOC concentration. Then, we developed a brand-new machine-learning model, hereafter entitled PARTYsoc AMG, linking the proportion of said stable SOC sensu AMG with the Rock-Eval® thermal analysis signature. Finally, we assessed the extent to which initializing the active and stable pool sizes of the AMG model using PARTYsoc AMG improved the agreement between measured and simulated stock values for 25 LTEs sites across the world.

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2 Materials and Methods

2.1 Experimental sites

The sites included in this study are LTEs having the data necessary for running classical soil C models, including the AMG model, and for which soil samples were available to be analyzed using Rock-Eval® thermal analysis. These are 25 agronomic LTEs involving treatments with contrasting levels of organic and mineral fertilization, straw management, crop rotations, bare fallow plots, etc. A brief description of the LTEs and the agronomic treatments is provided in Supp. Table 1, while a more detailed depiction of each site and the data necessary to run the AMG model are presented in a datapaper (Fujisaki et al., 2026). The geographic locations of the LTEs are shown in the interactive map (https://marija-stojanova.github.io/PARTYsoc-AMG-interactive-plots/map.html). Additionally, we have included the Boigneville site in France (Mary et al., 2020) whose data are available upon request. The code and data needed to run the model proposed in this work are made available as a Jupyter Notebook (https://github.com/marija-stojanova/PARTYsoc-AMG-publication-ready/blob/main/PARTYsoc_AMG.ipynb) and published in Stojanova et al. (2026).

2.2 Stable SOC stock optimization using the AMG model

The AMG model is a simple, mechanistic tool designed to simulate SOC dynamics in agricultural soils at a yearly time step (Andriulo et al., 1999). It divides SOC into two pools: an active pool with a mean turnover time of a few decades, and a stable pool considered inert over the simulation period of up to several decades (the stable carbon mineralization is considered negligible at this timescale). Carbon inputs, such as crop residues and organic amendments, are considered to be decomposed in one year, partly mineralized and partly feeding the active pool based on a mineralization coefficient depending on the type of fresh organic matter. The active SOC decomposition follows first-order kinetics, with rates controlled by climatic conditions and soil characteristics. In this paper, we used the AMG v2 model (Clivot et al., 2019).

Simulating the SOC dynamics of a given site requires configuring AMG with the initial SOC stocks of that site. These initial stocks are derived from the total measured SOC stocks, as well as a presumed initial SOC pool distribution. By default, the initial proportion of C in the stable pool (i.e., the stable SOC stock divided by the initial total SOC stock) depends on the historic land use of the site: 0.65 for sites with a long-term agricultural history (Saffih-Hdadi and Mary, 2008), and 0.40 for sites with a long-term grassland history (Huggins et al., 1998). We used the observed SOC dynamics at each site to optimize the stable SOC pool size. We did so by implementing the AMG v2 model detailed in Clivot et al. (2019) in Python and by using the scipy.optimize.minimize function and the BFGS algorithm (Virtanen et al., 2020) to minimize the root mean squared error (RMSE, see Equation 1) between the observed and predicted SOC stocks. A single optimal SOC stock is found for each site, meaning that sites with several different treatments have (potentially) different SOC proportions for each treatment. The optimization bounds are set as 10% of the minimum initial SOC stock across all treatments for the lower bound, and as 90% of the maximum initial SOC stock across all treatments for the upper bound. Exceptionally, if the upper bound is higher than

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the lowest initial SOC stock, then that stock is used as an upper bound. In some cases, we excluded treatments with more uncertain estimated carbon inputs from the optimization (e.g., treatments including perennial forage crops or those with cereals under low/nil nitrogen fertilization whose shoot-to-root ratios are different and thus the standard allometric functions cannot be applied). We assumed a non-convex objective function, and used basin hopping to avoid selecting a local minimum as the optimal value.

The optimized simulations were evaluated using the RMSE and the relative RMSE (RRMSE), defined as:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N} (y_i - \hat{y}_i)^2}, \quad (1)$$

and

$$RRMSE = RMSE / \underline{y}, \quad (2)$$

where N is the total number of samples, y_i is the observed value of the i-th sample, $\hat{y}_i$ its predicted value, and $\underline{y}$ is the mean of the observed samples.

After optimizing the stable SOC stock, the simulated stocks of the Rothamsted LTBF site did not accurately reproduce the observed dynamics (RRMSE > 10%). The resulting final SOC stock was significantly underestimated, confirming that a two-pool model cannot adequately account for the very rapid decline in SOC stocks following a long-term permanent grassland to bare fallow land-use change (Barré et al., 2010). We therefore truncated the beginning of this experiment and used a shorter time series (37 years instead of 49), allowing us to obtain more accurate simulations of SOC dynamics.

2.3 Rock-Eval® analysis

Our soil sample set included 641 topsoil samples from the 25 sites. All samples were air-dried or dried at 35 °C, sieved to <2 mm, and finely ground to <250 µm. They were then analyzed using a Rock-Eval 6® Turbo apparatus (Vinci Technologies). The samples were first pyrolyzed in an inert N2 atmosphere, then oxidized under purified ambient air (i.e., in presence of O2 and absence of CO2). The heating routine applied during pyrolysis started with a 3-minute isotherm at 200 °C followed by a heating ramp of 30 °C min−1 up to 650 °C. During the oxidation stage, an initial 1-minute isotherm was kept at 300 °C and followed by a heating ramp of 20 °C min−1 until 850 °C. The routine ended with a 5-minute isotherm at 850 °C (Barré et al., 2024; adapted from Behar et al., 2001).

The five resulting thermograms for each sample were processed using the Geoworks software (Geoworks V1.6R2, Vinci Technologies, 2021) resulting in 36 parameters. These parameters were then used as predictors by the PARTYsoc AMG machine-learning model. The full list of Rock-Eval® parameters and their definitions are provided in Supp. Table 2 (Delahaie et al., 2023). The TOCre6 and MINC values obtained using Rock-Eval® were corrected into SOCre6 and SIC to align with the data obtained through dry combustion elemental analysis, as described in Stojanova et al. (2024).

The response variable, representing each sample's stable SOC proportion, is obtained by combining the AMG-optimized per-site stable SOC concentration (Cs) and the SOCre6. The Cs concentration (in gC kg−1) is calculated as:

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$$C_s = \frac{C_{s,stock}[tC\ ha^{-1}]}{Soil\ mass\ [t\ ha^{-1}]} \times 1000\,, \quad (3)$$

160

from which we obtain each sample's stable SOC proportion (Cs,prop, unitless) as:

$$C_{s,prop} = \frac{C_s}{SOC_{re6}}. \quad (4)$$

2.4 Site and sample selection criteria

For each site, we tested the sensitivity of AMG simulations to changes in the initial stable SOC proportion. We compared the
165 absolute difference of the RRMSE obtained with the optimized initial stable SOC proportion and the one obtained when adding or subtracting 0.10 from this optimal value. Plotting these RRMSE values against the product of the simulated annual mineralization coefficient (k) and the LTE duration, we found a cluster of six sites insensitive to the initial stable SOC proportion, with an absolute difference in RRMSE < 0.02 (see Supp. Figure 1 and its interactive version). Low sensitivity to the initial stable SOC proportion is probably explained by the low amount of mineralized carbon at these sites during the
170 simulated period. The identified sites (Bretenière Res0Pest, Estrées-Mons SdC, Grignon SIC, KBS, Lanna and NELITCSE) have therefore a poorly-constrained stable SOC proportion, and their inclusion in the model significantly degraded the overall performance. These six sites were excluded from the learning set, but were nevertheless retained for the evaluation of PARTYsoc AMG. In total, the learning set contained Rock-Eval® results from 411 samples across 19 geographical sites. We tested different values for the sensitivity threshold, and found that the value of 0.02 is a good trade-off between the largest
175 possible training set and maximizing model performance. The performance metrics of an alternative model using an RRMSE threshold of 0.025 are shown in Supp. Figure 2 and its interactive version (https://marija-stojanova.github.io/PARTYsoc-AMG-interactive-plots/soc_validation_interactive_alternative_model.html), and details about this alternative model can be found in the Jupyter Notebook (Stojanova et al., 2026).

The samples retained in the learning dataset were unevenly distributed across the 19 sites, with some sites contributing fewer
180 than 10 samples and others more than 80. To prevent sites with larger sample sizes from disproportionately influencing the learned function, we imposed a limit of 15 randomly selected samples per site and per iteration (see Section 2.4.2). Potentially anomalous observations were identified using the Isolation Forest method (Liu et al., 2008), which detects outliers by recursively separating the data and measuring the path length to each observation. Observations that require an abnormally long path in order to be classified are seen as outliers. Approximately 5% of samples were marked as outliers and removed
185 from the learning set. Several combinations of values for the maximum number of samples per site and the percentage of outliers removed in the Isolation Forest procedure were tested to ensure the model is both robust and precise under varying parameters. The results are summarized in the accompanying Jupyter Notebook.

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2.5 Machine-learning model development

We employed a two-stage modeling strategy to predict the response variable. The first stage is a support vector machine (SVM), capturing nonlinear relationships between the predictors and the response. The second stage is a simple Beta regression, whose distributional assumptions guarantee predictions within the [0,1] interval. We used the SVM implementation provided in Python's scikit-learn library (Pedregosa et al., 2011) and the Beta regression from the statsmodels library (Perktold et al., 2024).

2.5.1 Model selection

SVMs are supervised learning algorithms that estimate relationships between a set of predictors and a response variable by finding an optimal function balancing model complexity with predictive accuracy (Brereton and Lloyd, 2010). While previous works modeling SOC dynamics have commonly relied on tree-based approaches, particularly random forests (RFs), we selected SVMs as they slightly outperformed RFs when applied to our dataset, specifically under independent validation (data not shown). While both RFs and SVMs are designed to model nonlinear and continuous relationships, they do so in very different ways. RFs mimic a continuous function by dividing the feature space into arbitrarily-small regions. SVMs implement kernels enabling truly continuous functions with regularization built into the model as a user-defined level of acceptable prediction error. This makes SVMs more easily generalizable, especially with small and medium size datasets. Unlike RFs, SVMs can extrapolate outside the response values seen in training and are less conservative near their distributional boundaries. However, this often makes SVM predictions less robust and stable than those of RFs, sometimes rendering truly implausible results. In our study, the addition of the Beta regression as a second step to the model, as well as a Mahalanobis distance criterion when applying the model to new data, allowed us to limit extrapolations in unobserved feature spaces.

2.5.2 Feature selection

The complete dataset included 36 Rock-Eval® features and the response variable Cs,prop. Feature elimination was initiated using the autofeatselect Python library, which we applied to remove highly correlated predictors and to rank them according to their predictive importance. Pairs of features with an absolute Pearson's correlation coefficient greater than 0.8 were considered highly correlated; in such cases, the feature less correlated with the Cs,prop was discarded. This procedure reduced the set to 15 out of the original 36 features. Subsequently, we ran 30 iterations of the autofeatselect algorithm to rank the 15 remaining features based on their permutation importance scores, using LightGBM as the estimator. Each iteration was trained on a different training subset due to the constraint of a maximum of 15 samples per site per iteration.

Our objective was to identify the smallest possible subset of features that maintained high predictive accuracy. Using the 15 retained features and their importance rankings, we determined the optimal feature set by running 30 iterations of cross-

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validated SVM training with subsets ranging from 2 to 15 features, ranked in the order of permutation importance. In each iteration, we ran both an internal training procedure and a leave-one-site-out (LOSO) procedure. In the LOSO procedure, 19 models were trained in every iteration, each excluding a single site from the training set, and subsequently applied to predict that site. In the internal validation procedure, one third of the data was systematically used as test data, allowing for validation on unseen samples. When selecting the optimal number of features, we aimed at maximizing the performance in LOSO validation, while ensuring that the model was not over-fitting in the internal validation. The selection criterion was the R2 coefficient of determination in LOSO (defined in section 2.4.3), and we applied the One standard error (1-SE) method that maximizes the R2 coefficient while minimizing the number of features used in the model (Breiman et al., 2017).

2.5.3 Training and validation

Once the features and the learning set were established, we proceeded with training one final model using the selected features. The final model, as well as all iterations of intermediary models, were cross-validated and we systematically checked for over-fitting by comparing training and test set performance metrics. These include the coefficient of determination (R2), the residual prediction deviation (RPD), the ratio of performance to interquartile distance (RPIQ), and the bias, defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^{N} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{N} (y_i - \underline{y})^2}, \quad (5)$$

$$RPD = \frac{SD}{RMSE}, \quad (6)$$

$$RPIQ = \frac{IQR}{RMSE}, \quad (7)$$

and

$$\text{Bias} = \hat{y} - \underline{y}, \quad (8)$$

where SD and IQR are the standard deviation of the observed values and their interquartile range (Q3 - Q1), and $\hat{y}$ is the mean of the predicted values.

With the final model established, we then used its predictions to initialize AMG's kinetic pools. We did so by calculating an average Cs concentration for each site, based on the predictions made for all its samples:

$$C_{s,PARTYsoc} = \frac{\sum_{n=1}^{N} \hat{C}_{s,prop}(n) \times SOC_{re6}(n)}{N}, \quad (9)$$

where $\hat{C}$s,prop(n) and SOCre6(n) and the predicted proportion of stable SOC and the Rock-Eval® measured SOC of sample n for a site with a total of N samples. The Cs concentration can then simply be transformed into the site's Cs,stock using Equation 3, and subsequently be used to initialize AMG. For sites where sampling was performed at multiple different depths, the equivalent soil mass (ESM) method was used in order to calculate a single Cs stock for the entire simulated soil layer, as described in Ferchaud et al. (2023).

https://doi.org/10.5194/egusphere-2026-6906
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2.5.4 Uncertainty and reproducibility

The reproducibility of the selected Rock-Eval® parameters, or their close equivalents, was studied by Pacini et al. (2023). We used their results to run Monte Carlo simulations by adding noise to the selected predictors, and thus estimate the uncertainty of the model. The noise levels added to predictors follow a Normal distribution whose parameters are reported by Pacini et al. (2023).

3 Results

3.1 Correlations between Rock-Eval® parameters and AMG-optimized stable SOC proportions

Using the AMG-optimized stable SOC stock values, we computed the optimal stable SOC concentration for each site and used it to calculate the Cs,prop of each sample. The stocks and concentrations of stable SOC obtained with AMG optimization are detailed in Table 1. Both the stock and concentration of stable SOC show significant variability, with values covering the range from 15.2 to 67.3 t C ha-1 and from 5.8 g C kg-1 to 15 g C kg-1, respectively. Table 1 also presents the range of variation of Cs,prop, i.e., the difference between the maximal and minimal Cs,prop for the samples of each site, and the number of samples for each site included in the learning set. The variation in the proportion of stable SOC significantly differs between sites, with some having absolute differences of around 10 percentage points (e.g., Folleville or Bad Lauchstädt LTBF), and others having over 50 percentage points difference between the maximum and minimum stable SOC proportions (e.g., Boigneville, Lönnstorp, Pergamino, Rothamsted LTBF, Versailles La Cage, Versailles LTBF).

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Site	C_s stock (t C ha^{-1})	C_s concentration (g kg^{-1})	Number of samples	$C_{s,prop}$ min	$C_{s,prop}$ max	Soil depth (cm)
Askov LTBF	31.0	10.4	7	0.60	0.83	20
Bad Lauchstädt LTBF	57.3	15.0	16	0.78	0.90	30
Boigneville	26.5	6.7	68	0.31	0.93	28
Estrées-Mons Res0Pest	26.1	8.8	8	0.64	0.78	30
Fagnières LTBF	29.6	9.6	16	0.53	0.81	25
Feucherolles Qualiagro	29.0	7.2	19	0.50	0.84	28
Folleville	34.9	10.0	15	0.74	0.84	30
Grignon LTBF	16.5	8.3	16	0.58	0.89	25
Issoudun	28.8	12.2	16	0.70	0.83	23
Kerbernez	52.5	12.8	38	0.45	0.73	25
Lönnstorp	28.3	9.2	19	0.45	0.96	23
Lusignan ACBB	31.3	7.1	10	0.48	0.74	30
Mant	25.0	7.1	16	0.63	0.91	28
Pergamino	32.5	11.9	34	0.34	0.95	26
Rothamsted LTBF	28.8	8.8	13	0.21	0.89	23
Ultuna	27.7	5.8	85	0.28	0.68	20
Versailles La Cage	26.2	7.1	20	0.31	0.80	30
Versailles LTBF	28.0	7.0	7	0.39	0.91	25
Waite	15.2	12.2	7	0.43	0.90	10

Table 1: Summary of the learning dataset. Cs stock and Cs concentration are the optimal stock and concentration per site as found in AMG simulation.

Figure 1 shows the correlations between AMG optimal stable SOC proportions and various common Rock-Eval® parameters for each site and for all sites combined. Strong and significant correlations are found with several Rock-Eval® parameters even when the samples from all sites are combined, notably for the T50-CO2OX and T50-CO2PYR. On a per-site basis, the T50-CO2PYR had an overall strong positive correlation with the target CS,prop, with the exception of two sites whose correlations generally do not follow the established trends (Feucherolles Qualiagro and Mant). To a lesser extent, general correlations exist between the combined data and the oxygen (OIre6) and hydrogen index (HI), as well as the two temperature parameters monitoring the hydrocarbon effluents during pyrolysis (T50-HCPYR and T90-HCPYR). While the HI correlations

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are generally negative and consistent, the OIre6 and T50-HCPYR correlations are generally positive, but with several exceptions.

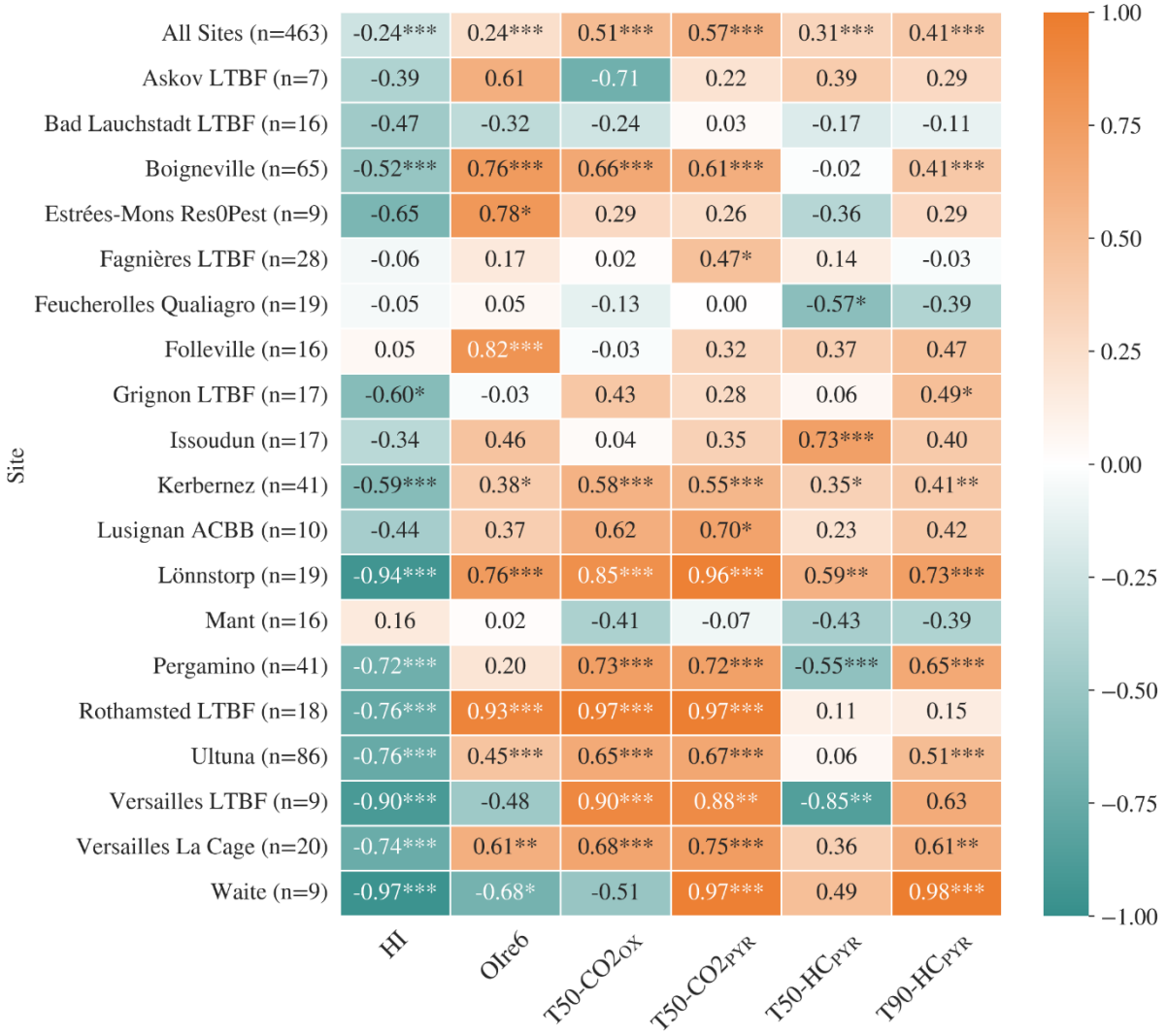

Figure 1: Correlations between AMG optimal stable SOC proportion (Cs,prop) and main Rock-Eval® parameters for each site and for all sites combined. Significance levels are indicated as: * = p < 0.05, ** = p < 0.01, *** = p < 0.001, and are calculated using Spearman's r.

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3.2 Predicting the proportion of AMG's stable SOC pool size

We used 463 samples from the 19 selected sites to build the PARTYsoc AMG machine-learning model. The selected model used six Rock-Eval®-based features: SOCre6, T50-CO2PYR, T50-HCPYR, T90-HCPYR, HI, T10-COOX. The features SOCre6 and HI correspond to the SOC measured by Rock-Eval® and the amount of pyrolysis effluents divided by the TOCre6, respectively. The other Rock-Eval® variables depend on the shape of the thermograms. TX-Y corresponds to the temperature at which heating is required to recover X% of the signal from the Y thermogram. Interestingly, the SVM model retained information coming from three different thermograms (HC and CO2 signals in pyrolysis, and CO in oxidation). The results of the feature selection procedure and the performance metrics are shown in Supp. Figure 3 and Supp. Table 2.

Figure 2 shows the internal validation (Figure 2a) and independent validation (Figure 2b) of the selected model. An interactive version is available here (https://marija-stojanova.github.io/PARTYsoc-AMG-interactive-plots/soc_validation_interactive.html). The internal validation metrics showed no bias and had satisfactory RPD and RPIQ values higher than 2. As anticipated, the LOSO metrics were lower, yet still highly satisfactory (no bias, RPD and RPIQ >1.7).

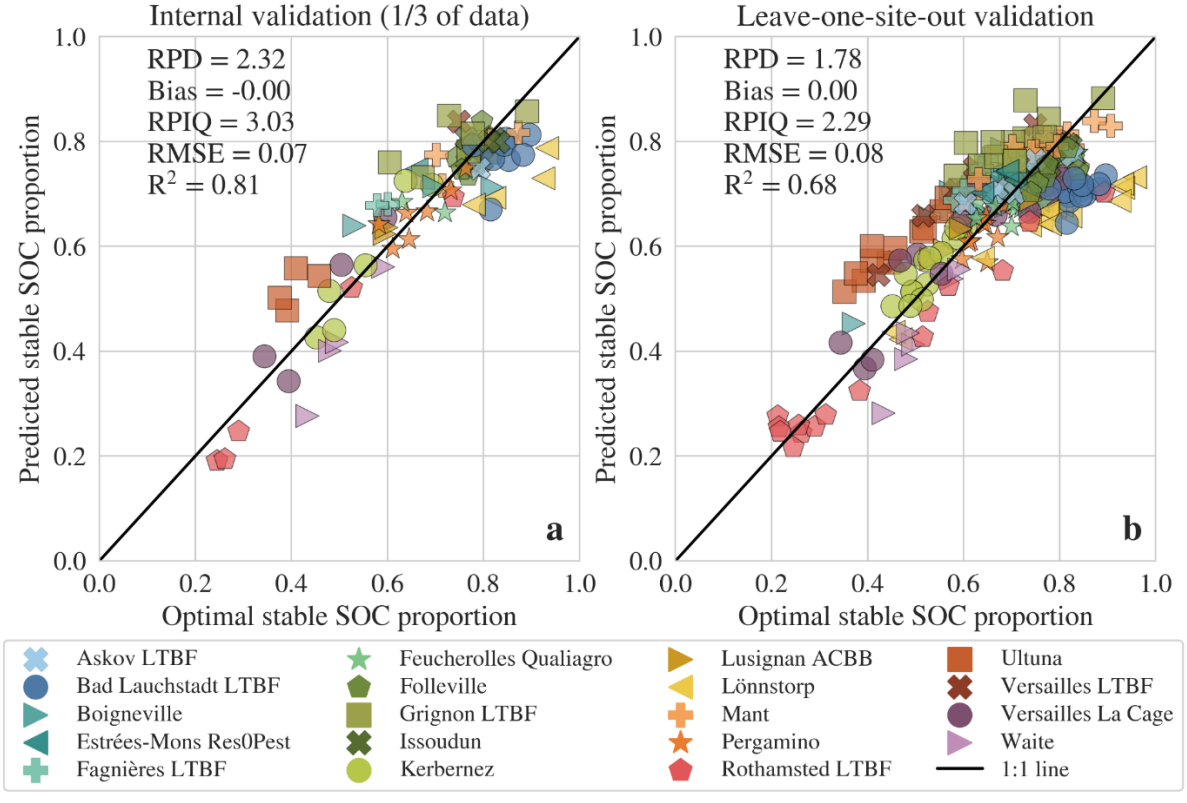

Figure 2: Predicted AMG optimal stable SOC proportion calculated using PARTYsoc AMG plotted against optimal AMG stable SOC proportion. Figure 2a presents the internal validation and Figure 2b the LOSO (independent) evaluation.

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3.3 Comparison of AMG simulations accuracy for different kinetic pool initializations

Figure 3 compares the average RMSE of the AMG simulation for each site when partitioning between the active and stable SOC pools was performed using the optimal value, the default value, or the value provided by the PARTYsoc AMG model. The results are presented for the 19 sites included in the training set and the 6 sites (for which the initialization had little effect on the simulation of SOC changes) used for the validation only. For the majority of the 25 sites, PARTYsoc AMG initialization decreases the RMSE compared to the default initialization. The highest differences resulted in a decrease from 6 t C ha-1 to 2 t C ha-1 of the mean RMSE (Ultuna, Grignon LTBF, Versailles LTBF, Bad Lauchstadt LTBF, Kerbernez, Pergamino). For some sites, the PARTYsoc AMG initialization did not improve the quality of simulations compared to default initialization. However, with the exception of Bretenière Res0Pest, the use of PARTYsoc AMG never significantly degraded the quality of simulations. Moreover, sites for which the use of PARTYsoc AMG is not beneficial already have very low RMSE values when using the default initialization. Off note, the Bretenière Res0Pest site has only three sampling dates and the largest absolute standard deviation in the dataset, thus its results should be interpreted with caution.

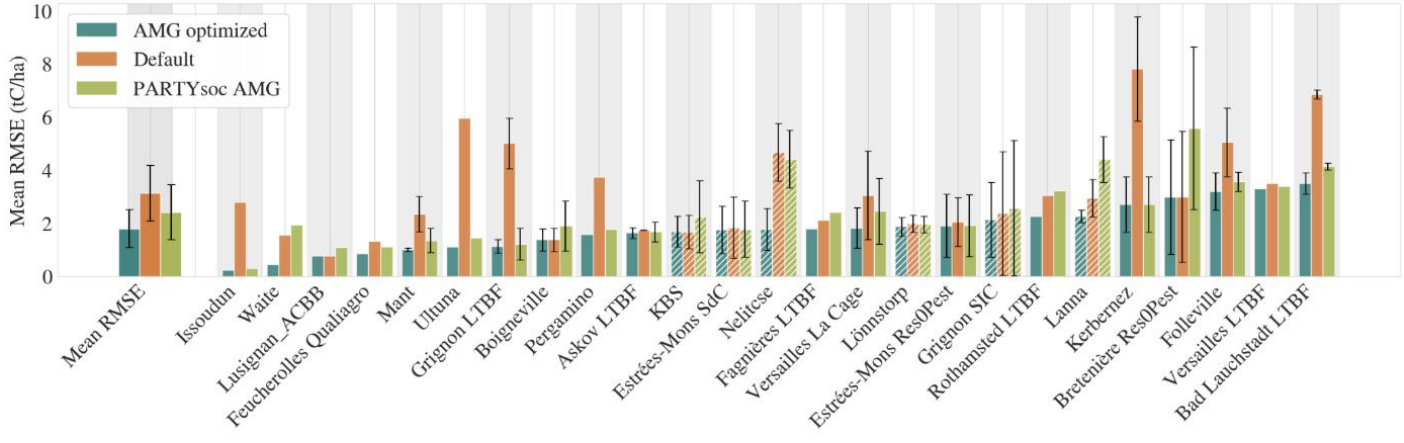

Figure 3: Comparison of the average RMSE per site for AMG simulations when the model was initialized using the optimal stable SOC proportion, the default proportion, or the proportion provided by PARTYsoc AMG. Bars with hatching indicate the six sites not used in the training set. The error bars indicate the standard deviation when several treatments are present in a site.

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4 Discussion

4.1 Rock-Eval® parameters as indicators of SOC biogeochemical stability

By applying an inversion-based optimization on the dataset comprising 463 soil samples collected across 19 worldwide temperate LTE sites, we have found the optimal SOC pool size of each site, as defined by the AMG model. These results allowed for the calculation of a sample-wise stable SOC proportion and, consequently, an estimation of SOC biogeochemical stability (Table 1). Rock-Eval® thermal analysis was used to assess the elemental stoichiometric composition and thermal stability of organic matter. In agreement with previous observations on smaller datasets (Gregorich et al., 2015; Barré et al., 2016; Cécillon et al., 2018; 2021; Poeplau et al., 2019; Mesgar et al., 2025), these results confirm the link between SOC thermal and biogeochemical stability. A positive correlation between the Cs,prop and the temperature parameters T50-CO2PYR, T90-HCPYR, and T50-CO2OX is observed for nearly all LTEs. However, the correlation with T50-HCPYR is generally weaker, with several sites even exhibiting significantly negative relationships (Figure 1). This result is in line with a previous study on French agricultural and forest soils suggesting that T50-HCPYR is a poorer indicator of SOC biogeochemical stability compared to T50-CO2PYR, T90-HCPYR, and T50-CO2OX (Delahaie et al., 2023).

Overall, the Rock-Eval® thermal analysis shows that, on average, OM with higher biogeochemical stability (higher Cs,prop) is more oxidized (higher OIre6 which is a proxy for O/C ratio), while less biogeochemically stable organic matter is more prone to reduction (higher HI which is a proxy for H/C ratio). The oxidation state of organic matter could provide a thermodynamic explanation for its biogeochemical stability. In an oxic environment, like the cropland soils considered in the study, more energy is generated when oxidizing reduced OM (La Rowe and van Cappellen, 2011). The lower stability of high-HI organic matter could therefore be explained by the fact that it constitutes a better energy source for microorganisms. However, some LTEs have a significantly negative correlation between OIre6 and biogeochemical stability, contrary to both the general tendency of most LTEs and the average correlation observed over the entire dataset (Figure 1). Interestingly, these sites likely have higher concentrations of pyrogenic C than the others: Versailles LTBF contains a significant amount of char (e.g., Chassé et al., 2021), Bad Lauchstadt is a Chernozem, and Waite is an Australian site, a region where fire history has been extensively documented. Pyrogenic C is characterized by having both a low HI and a low OI. For these sites, it is likely that a higher proportion of stable C is accompanied by a higher proportion of pyrogenic C. As a result, the more biogeochemically stable OM is enriched in pyrogenic materials with a very low OI, leading to a negative correlation between biogeochemical stability and OI for these specific sites. These results suggest that the relationship between biogeochemical stability and OIre6 should be interpreted with caution, especially for sites rich in pyrogenic C.

4.2 PARTYsoc AMG predictions provide accurate kinetic pool initializations

Our data establish a substantial and consistent relationship between the Rock-Eval® thermal analysis results and SOC biogeochemical stability, confirming the possibility to develop multivariate models that predict biogeochemical stability based solely on Rock-Eval® measurements. Unlike previous studies (Cécillon et al., 2018; 2021), stable carbon quantities were

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obtained by optimizing a SOC dynamics model and are not directly derived from observed SOC decline in long-term bare fallow sites. As a result, Cs quantities could be estimated across a larger number of sites (19 vs. 7), thereby expanding the training dataset. However, this calculation of Cs quantities also incorporates potential errors of the AMG model.

We compared the performance of several different machine-learning models and selected a combined SVM + Beta regression model that provided the highest accuracy (Figure 2) with the lowest overfitting (Supp. Fig 2). The internal validation metrics were similar to those obtained with the PARTYsoc v2.0 model (Cécillon et al., 2021), but the results show a significant improvement in LOSO validation, with a reduction in RMSE from 0.15 to 0.08. Moreover, the proposed model uses only six Rock-Eval® parameters, compared to its predecessor that incorporates 18 parameters. Interestingly, among all the available Rock-Eval® parameters, the selected model uses predictors from thermograms obtained during the pyrolysis and oxidation phases. This illustrates that 1) the information linking Rock-Eval® results and SOC biogeochemical stability comes from different thermograms, and that 2) the use of thermal methods involving only a pyrolysis phase or only an oxidation phase would probably not yield results of the same quality. It should be noted that the extrapolation capabilities of SVM models, unlike those of RF models, render their application potentially more risky outside the learned application domain. Thus, we advise a systematic check of suitability when applying the proposed PARTYsoc AMG model on new data by calculating a Mahalanobis distance criterion detailed in the Jupyter Notebook (https://github.com/marija-stojanova/PARTYsoc-AMG-publication-ready/blob/main/PARTYsoc_AMG.ipynb) and published in Stojanova et al. (2026).

On average, using PARTYsoc AMG to initialize the sizes of the stable and active pools in AMG simulations improves the agreement between simulated and observed SOC stock changes (Figure 3). The mean RMSE across all sites was 3.14 t C ha-1 with the AMG default initialization, and it decreased to 2.41 t C ha-1 with PARTYsoc AMG initialization, and 1.81 t C ha-1 with optimized initialization, corresponding to RRMSE of 8.4%, 5.2%, and 3.9%, respectively. The general performance obtained over the 25 sites with the PARTYsoc AMG initialization was higher than that obtained previously in arable temperate sites with the default AMG initialization: RMSE of 2.6 t C ha-1 (5.3%) for 20 sites (Clivot et al., 2019), RMSE of 2.8 t C ha-1 (10%) for 7 sites (Levavasseur et al., 2020), or RRMSE = 7.5% for 6 sites (Farina et al., 2021). These results show that 1) the default initialization of the AMG model, at first order, correctly reproduces SOC stock dynamics in temperate arable soils, 2) the use of a PARTYsoc AMG initialization further improves the model's performance, and 3) this performance will be difficult to further surpass as it is of the order of magnitude as the SOC stocks measurement error.

4.3 PARTYsoc AMG: A new perspective for SOC model initialization

The method proposed here resolves the decades-long issue of accurately initializing AMG's kinetic pool sizes. We have shown that using PARTYsoc AMG makes it possible to simulate changes in SOC stocks for 25 worldwide temperate sites with remarkable accuracy. The initialization method developed currently only applies to the AMG model. However, the methodology could be generalized to other compartmental models simulating SOC stock dynamics. Using this publicly available dataset (Fujisaki et al., 2026), one can find the data-driven optimal initial kinetic pool sizes in other models. It would then be possible to determine the proportion of SOC in the different pools for each sample and use this information to train

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machine-learning models linking the proportions in the different pools to Rock-Eval® thermal analysis data. However, this procedure would need to be adapted for models with more than two kinetic pools, particularly when some pools have similar mean residence times (MRTs). For example, in the RothC model (Coleman and Jenkinson, 1996), three of the five pools ("microbes", "decomposable plant materials", and "resistant plant materials") have MRTs ranging from 1 to 10 years. Without proper adjustment of the method, the presence of compartments with comparable MRTs will cause equifinality issues, making pool size optimizations too uncertain.

Nonetheless, our approach offers the clear prospect of finally resolving the nagging question of initializing the sizes of conceptual pools (Christensen, 1996; Elliott et al., 1996). By adopting a hybrid AMG approach, it becomes possible to retain the operational simplicity of compartmental models while simultaneously avoiding the difficulties associated with initializing the conceptual pools' sizes. In this regard, PARTYsoc AMG is a clear paradigm shift that allows for more accurate simulation of absolute changes in SOC stocks, which should have significant implications for the estimates of potential cropland SOC contributions for nationally determined contributions, voluntary C market regulation, or evaluations of agricultural and environmental policies.

The current version of PARTYsoc AMG has been developed using data from 19 LTE sites and evaluated on 25 sites. These sites cover a wide range of soil and climatic conditions mainly for temperate zones, rendering the model widely applicable in temperate agrosystems and potentially adaptable to other contexts. Thus, it would be very useful to test the model on new sites in other temperate regions and, even more so, on data collected in tropical areas to increase its area of applicability. Both the improvement and the generalization of the proposed initialization procedure are highly dependent on the persistent and rigorous development of databases providing data from different sites having available archive samples for Rock-Eval® characterization. As PARTYsoc AMG is a learning model, the arrival of new data would initiate a virtuous circle of continuous improvement. Such a collective effort, grounded in a genuine willingness to share data, would represent a major step toward developing SOC models that can meaningfully contribute to reliable global carbon crediting.

5 Conclusion

Accurately quantifying soil organic carbon (SOC) dynamics remains central to understanding and quantifying the impact of agricultural practices on soil health and the global carbon cycle, and to evaluating mitigation strategies in the context of climate change. In this study, we developed a data-driven model for predicting SOC dynamics in temperate agricultural soils that combines high predictive performance with a parsimonious set of inputs. Our results show that this model achieves high predictive accuracy (RMSE = 0.08 in leave-one-site-out validation), and can be used to improve the initialization of the AMG model, reducing its prediction error by 30% relative to default parameterization.

Beyond predictive performance, our findings demonstrate that a small set of Rock-Eval® thermal indicators can be used as a proxy for SOC biogeochemical stability within the AMG modeling framework. In the context of ongoing efforts to develop and share harmonized SOC datasets, this study provides a practical solution to the longstanding challenge of initializing

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conceptual carbon pools in SOC models of similar complexity to AMG. Finally, extending this and similar datasets across a wider range of pedoclimatic conditions will be essential to the assessment of the generality of these relationships and to develop more robust and widely applicable SOC models.

Data and code availability. The data and code supporting this study are openly available as a Zenodo repository at https://doi.org/10.5281/zenodo.18799111.

Supplement link.

Author contribution. Marija Stojanova: conceptualization, data curation, formal analysis, software, investigation, methodology, visualization, writing – original draft, writing – review and editing. Fabien Ferchaud: conceptualization, data curation, resources, formal analysis, funding acquisition, investigation, methodology, writing – review and editing. Hugues Clivot: conceptualization, data curation, resources, formal analysis, investigation, methodology, writing – review and editing. Lauric Cécillon: conceptualization, data curation, investigation, methodology, writing – review and editing. Andrian Andriulo: data curation, resources, writing – review and editing. François Baudin: data curation, resources, writing – review and editing. Claire Chenu: data curation, resources, writing – review and editing. Bent Christensen: data curation, resources, writing – review and editing. Kenji Fujisaki: data curation, writing – review and editing. Thomas Kätterer: data curation, resources, writing – review and editing. Florent Levavasseur: data curation, resources, writing – review and editing. Ines Merbach: data curation, resources, writing – review and editing. Christopher Poeplau: resources, writing – review and editing. Jonathan Sanderman: data curation, resources, writing – review and editing. Pierre Barré: conceptualization, formal analysis, funding acquisition, project administration, investigation, writing – original draft, writing – review and editing.

Competing interests. The contact author has declared that none of the authors has any competing interests.

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field experiment is part of the SOERE-PRO (network of long-term experiments dedicated to the study of impacts of organic waste product recycling) integrated as a service of the "Investment in the Future" infrastructure AnaEE-France, overseen by the French National Research Agency (ANR-11-INBS-0001). The Qualiagro experiment was founded and is still supported by INRAE and Veolia. The Versailles LTBF and Versailles La Cage experiment were founded by and are still supported by INRAE. TK received funding from FORMAS (grant no. 2022-00214).

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