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Reply on RC1

Lauric Cécillon et al.

Author comment on "Partitioning soil organic carbon into its centennially stable and active fractions with machine-learning models based on Rock-Eval® thermal analysis (PARTY_{SOC}v2.0 and PARTY_{SOC}v2.0_{EU})" by Lauric Cécillon et al., Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2021-16-AC1>, 2021

Reply to reviewer 1 (Dr. E. Lugato)

R1: The authors present an improved version of a method previously published (Biogeosciences, 15, 2835–2849, 2018), combining thermal analysis and machine learning in order to predict a centennial stable and active soil organic pool. It is certainly an interesting approach, that can provide useful indications for monitoring soil organic carbon and quality changes. The methodology is amply described as well as the validation process, therefore, I have only minor recommendations.

Reply: we deeply thank Dr. Lugato (reviewer 1) for his positive feedback on our work and manuscript (MS).

R1: Personally, I would be more careful in recommending the application of PARTY_{SOC}v2.0_{EU} in European agricultural topsoils (line 43), since the performances were lower both in the 'leave-one-out-site' and in the two independent sites validation. This is an indication that PARTY_{SOC}v2.0_{EU} would benefit of additional training sites; due to great variability of pedo-climatic and agroecosystem conditions in Europe, application of machine learning methods outside the range of their training can be critical.

Reply: we fully agree with Dr. Lugato and also with reviewer 2 (see our reply to reviewer 2) that the application of machine-learning models outside the range of their training set cannot be recommended.

We accordingly revised the main text, specifying that "*To this respect, we consider that applying the second version of PARTY_{SOC} to unknown soils from pedoclimates outside its training set cannot be recommended*" (lines 607–608 of the revised MS). We also revised the abstract accordingly, removing our overoptimistic recommendation highlighted by Dr. Lugato and also by reviewer 2. We further refined the text of the abstract with the following sentence: "*More specifically, our results show that PARTY_{SOC}v2.0_{EU} reliably partitions SOC kinetic fractions at its Northwestern European validation sites on Cambisols and Luvisols, which are the two dominant soil groups in this region*" (lines 41–42 of the revised MS). This refined statement is based on new results of the model (sensitivity analysis to the test set) presented at lines 527–532 of the revised MS, and in the new supplementary Figure S1.

R1: Also the discussion presents, sometime, some repetitive concepts.

Reply: we thank Dr. Lugato for this comment. We significantly revised the Discussion section of the MS. First we tried to avoid repetitions (we shortened the Sections 4.2 and 4.3, removing a full paragraph from Section 4.3); second we refined the discussion paragraphs related to the applicability of PARTY_{SOC}V2.0_{EU} in European agricultural topsoils, as meaningfully recommended by both Dr. Lugato and reviewer 2 (see our reply to reviewer 2).

R1: I would also have expected more about comparison with other approaches especially in term of cost-benefit. While this method can be applied on existing monitoring schemes (as it requires a soil sample), there is no information of the cost of the thermal analysis, the complexity etc., which are interesting aspects if the aim is to propose a routine method.

Reply: we thank Dr. Lugato for his meaningful suggestion. We added in the main text some information regarding the cost of Rock-Eval® thermal analysis: "*These characteristics are measurable quickly (ca. 1 h per sample) and at a reasonable cost (less than 60 USD per sample in private laboratories) using Rock-Eval® thermal analysis*" at lines 100–102 of the revised MS.

R1: Line1: I would suggest adding in brackets after 'active' (with turnover time of months to a few years).

Reply: In our work, we are referring to a centennially active soil organic carbon (SOC) fraction, which means that it has a typical mean turnover rate of a few decades. To clarify this point, we modified the corresponding sentence in the abstract "*stable or active on a century scale*" (line 28 of the revised MS). Information related to this point is also provided in the main text: "*The most drastic conceptual simplification of SOC persistence considers only two pools: (1) one made of young SOC with a short turnover rate (typically three decades on average; the active SOC pool) and (2) one made of older SOC that persists much longer in the soil (more than a century; the stable, passive or persistent SOC pool)*" (lines 61–64 of the revised MS).

R1: Line 77-80: it seems that the approach proposed is quite insensitive to the number of samples training the model. Indeed only 7 sites are used and the 'leave-one-site-out' validation is worse than the 'internal'. This is a likely sign that also this model would benefit from additional training. So I don't understand the concept that other methods 'need to be inferred from statistical models or infrared spectroscopy'. Isn't it also what the authors are doing, training a ML on measurements?

Reply: we agree with Dr. Lugato that the PARTY_{SOC} model would benefit from additional training sites, as already stated in the discussion section, see e.g. "*The very first future improvements to the PARTY_{SOC} machine-learning model are to increase the size and further expand the pedoclimatic diversity of its training set*", at lines 625–626 of the revised MS.

At lines 76–81 of the revised MS, we are actually addressing a different point, i.e. that only a few techniques are "*reasonably reproducible and easy to implement such as the ones based on rapid thermal analysis and chemical extractions*" compared to other techniques such as the tedious "*size and density SOC fractionation*" methods. On the other hand, we recognize that the technical difficulties in implementing size and density SOC fractionation methods on large soil sample set can be resolved by inferring their results from regression models based on environmental variables (e.g. Cotrufo et al., 2019) or infrared spectroscopy (e.g. Viscarra Rossel et al., 2019).

We would like to point out that such works are using machine-learning in a way that differs from our approach. Our approach uses machine-learning to link Rock-Eval® parameters to long-term observations of soil carbon persistence, but it always requires the use of a Rock-Eval® measurement to infer soil carbon pool partitioning in a new soil sample. This is not the case for the approaches of e.g. Viscarra Rossel et al. (2019) or Cotrufo et al. (2019) that use machine-learning with the only goal of avoiding the use of tedious physico-chemical soil carbon fractionation methods on numerous soil samples. These approaches then predict, using only infrared spectroscopy or environmental information that are available from new soil samples or new sites, the size of different soil carbon fractions corresponding to a mixture of centennially stable and active carbon, as illustrated in our conceptual Figure 1.

R1: Line 82. I generally agree, although I would like to point out that some fractionation methods don't necessary aim at isolating kinetically defined pools, but rather pools underlying pathways of SOC formation and stabilization (e.g. the work on MEMS by Cotrufo et al.).

Reply: we agree with Dr. Lugato that some fractionation methods may aim at isolating pools with specific formation, stabilization and destabilization process, but we first note that most of these attempts have proven to be unsuccessful (von Lützow et al., 2007). Second, when it comes to modeling soil carbon dynamics, isolated soil carbon fractions are usually transformed to conceptual kinetic pools with a unique decay rate, which is not correct since the isolated fractions are most often a mixture of fast-cycling and slow-cycling carbon (von Lützow et al., 2007). This is the case of the MEMS model that is "*directly equating mineral-associated organic matter and particulate organic matter fractions with corresponding model pools*" (Robertson et al., 2019), assigning a unique decay rate for the particulate or the mineral-associated fractions.

R1: Lines 85-86: yes, unless models are built to predict model fractions (eg. MEMS, COMISSION and others)

Reply: we agree with Dr. Lugato that models are meaningful to test competing theories on soil carbon dynamics. On the other hand, it seems obvious from the literature that models of SOC dynamics such as the MEMS model are not built for the sole purpose of predicting model fractions. Clearly, the MEMS model was built to forecast soil organic carbon dynamics "*it does provide the basis for a more mechanistic model that can simulate SOM dynamics on the ecosystem scale*" (Robertson et al., 2019).

R1: Fig.1 left panel. Is it a conceptual figure or size fractions were effectively analyzed by RockEval?

Reply: Figure 1 is a conceptual figure illustrating that all soil carbon fractionation methods (e.g. size-based methods, thermal methods, etc.) are consistently isolating fractions that are a mixture of centennially stable and active carbon. In this Figure, we state that is only when calibrated on long-term observational data of SOC persistence (as done by the PARTYSOC machine-learning model) that fractionation methods such as Rock-Eval® thermal analysis can reliably quantify the respective sizes of the centennially stable and active SOC fractions. For information, some Rock-Eval® measurements of soil carbon size or chemical fractions are reported in previously published papers (Saenger et al., 2015; Soucémarianadin et al., 2019; Poeplau et al., 2019).

R1: Line 195: It seems that authors suggest that the lowest SOC treatment received less 'unwanted' C input, while its lower value may be due to any source of uncontrolled variability. Are the results very sensitive to this approach and is there any risk to, opposite, underestimate the centennial carbon pool?

Reply: we thank Dr. Lugato for this comment. We agree that a value of total SOC content lower than the site-specific estimate of the centennially stable soil carbon content may indicate an uncontrolled within-site variability of the soil carbon content (and of the centennially stable carbon content). However, we consider that the risk of overestimating the centennially stable soil carbon content using the curve-fitting method proposed by Barré et al. (2010) is much higher (as stated at lines 190–196 of the revised MS) than the risk of underestimating it using the modified methodology proposed in our MS. This is best illustrated at the site of Rothamsted (England), where the lowest total SOC measurement (9.72 gC/kg) is lower than our curve-fitting estimate of the centennially stable carbon content at that site (10.46 gC/kg; Cécillon et al., 2018), while this value (retained as the more accurate site-specific value of centennially stable soil carbon content, see Table 1) remains much higher than another estimate of the centennially stable soil carbon content (7.9 gC/kg) reported for another bare fallow experiment at the same site and for the same soil type by Jenkinson and Coleman (1994; see the Discussion section at lines 614–623 of the revised MS).

R1: Line 275: maybe 'inferred' is better than 'calculated' as a fitting procedure was generally used.

Reply: "calculated" was replaced with "inferred" at lines 274 and 276 of the revised MS.

R1: Table 1: while the Centennial stable SOC is a unique value per site, what does the SOC content refer to (average over all treatments and years within a site)?

Reply: we thank Dr. Lugato for this comment; the basic statistics of SOC content reported in Table 1 refer to the reference soil samples used (15 per reference site). We clarified this point in the revised version of Table 1.

R1: Line 358: if I well understood, out of those 105 samples, the centennial stable pool was inferred only from the LTBF and, then, assumed to be the same for all other treatments within the same site. I was wandering if some agronomic practices (for instance organic application) can bias this assumption. In fact, as far as understood (line 315), treatments with repeated application of some types of exogenous organic matter were not considered. My question is whether this poses a limit in the wide applicability of the method, since lot of soils receive manure and compost in Europe.

Reply: we thank Dr. Lugato for his comment and question regarding the influence of exogenous organic matter (EOM) applications to soil on its centennially stable carbon content.

While this is beyond the scope of the present work, we agree that the question raised by Dr. Lugato is important. As stated at lines 312–320 of the revised MS, we suspect that repeated applications of EOM to soil may increase the content of the centennially stable SOC fraction after several decades (e.g. biochar).

However, we would like to point out that such effects of repeated EOM applications on the centennially stable soil carbon content only impacts the selection of reference sites for the PARTY_{SOC} machine-learning model (as explained in details at lines 312–320 of the revised MS), but that these effects do not affect the applicability of our method on unknown soils (as long as the PARTY_{SOC} machine-learning model is able to capture these effects).

R1: Table 2. Adding one site (La Cabana), the rank of the variable importance changed as well as the predicted centennial SOC proportion on a different extent depending on sites (Fig. 2b, Fig. 3a,b). Have authors considered to introduce

additional variables in the Random Forest model (eg. texture) to make it more robust?

Reply: we thank Dr. Lugato for this meaningful comment. The current version of the PARTY_{SOC} machine-learning models is based on a limited number of reference sites and is thus, in its current configuration, sensitive to the addition of new sites, as illustrated by the results of the sensitivity analysis to the training set, presented in Figure 3 and in the supplementary Table S5.

We agree with Dr. Lugato that adding predicting variables, such as soil texture, could potentially improve the performance and the robustness of the PARTY_{SOC} machine-learning model. However, as stated above, the model is currently based on a limited number of reference sites, and we think that adding soil and environmental properties as predicting variables may, on the other hand, reduce the robustness of the model when applied to new sites. This option is nevertheless under consideration for the next version of the model that will integrate a significant number of additional reference sites in its training set.

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