

The results presented by Stojanova et al. (2024) constitute a significant contribution to the use of Rock-Eval thermal analysis in soil science, as they provide the first comparative study of correction methods for organic carbon (Corg) and inorganic carbon (Cinorg) contents measured by RE in soil samples.

This question is highly relevant because, from the first RE applications to soil samples, Disnar et al. (2003) already observed a significant discrepancy between organic carbon (Corg) contents measured by RE (TOC parameter) and by elemental analysis (LECO). These authors then proposed an "empirical correction" based on simple linear regressions between RE and LECO measurements using a dataset (n = 100) representative of the main types of horizons (organic, organo-mineral, and mineral) sampled under contrasting pedoclimatic conditions.

The manuscript presented by Stojanova et al. (2024) certainly addresses the shortcomings of this initial approach. Firstly, the authors clearly formalize their objectives to minimize discrepancies between organic carbon (Corg) and inorganic carbon (Cinorg) contents by using elemental measurements as a reference. Secondly, the study is conducted on a large panel of samples (n = 240) covering a wide range of Corg (0-50 g.kg<sup>-1</sup>) and Cinorg (0-80 g.kg<sup>-1</sup>). Thirdly, the study involves comparing the performances of several models using objective statistical criteria. Results show that these performances, analyzed for different soil categories, allow the identification of a significantly more efficient model than others, thus providing a simple and effective post-analysis "statistical correction" for the studied soil types.

Reading the manuscript, however, raises some incidental questions that can be shared with the authors to strengthen this technical note.

*Answer : thanks for your positive feedbacks and interesting comments.*

Among the correction procedures tested by Stojanova et al. (2024), four are proposed by the authors, while the fifth is presented as a "correction model" proposed by Hazera et al. (2023), which constitutes a shortcut and raises an attribution issue. Indeed, the work presented by Hazera et al. (2023) focuses exclusively on adjusting the Rock-Eval analytical protocol to improve the accuracy of the initial measurement. The question of post-analysis corrections is addressed as a technical contingency based on the literature. In the "Materials & Methods" section, Hazera et al. (2023) present the empirical correction protocol proposed by Disnar et al. (2003), and then another protocol of "parametric correction" based on a prior interpretation of the RE data (Sebag et al., 2022). Hazera et al. (2023) explicitly state that they use the empirical parameters proposed by Disnar et al. (2003) to correct RE measurements. Therefore, by adopting the protocol used by Hazera et al. (2023), Stojanova et al. (2024) compare the performances of their statistical models to the empirical procedure proposed by Disnar et al. (2003). It seems important to correct this attribution error to avoid any confusion regarding the origin of the correction method.

*Answer : the correction proposed in Hazera et al. comes from Disnar et al. and SOTHIS. As the description of the SOTHIS correction refers to a patent, it is not easy to find. For this reason, we refer to Hazera et al., as the full correction method (Disnar + SOTHIS) is clearly explained only in this article. We will make it clearer in the revised version. Moreover, our work also confirms that all carbonates have evolved as CO<sub>2</sub> using the classical "sol" mode of the Rock-Eval(r) (described in detail in Cécillon et al., 2018) and that the adjustment of the usual analytical protocol is not necessary.*

By using the formulas presented by Hazera et al. (2023), Stojanova et al. (2024) implicitly employ the empirical correction procedure proposed by Disnar et al. (2003) without explicitly

stating it. However, this procedure explicitly comprises two distinct and successive steps: the first applies unconditionally to all samples, while the second applies only under certain conditions to specific samples after a prior examination of qualitative RE parameters. In the present form of the manuscript, it appears that Stojanova et al. (2024) systematically applied the second step to all samples without prior verification of the conditions for its application. It is crucial that the procedure proposed by Disnar et al. (2003) is implemented in accordance with its technical recommendations. It is highly likely that the results will not be radically different from those currently presented, but it will minimize any uncertainty when comparing the models' performances.

*Answer : There is indeed a different correction to apply depending if one considers that the soil samples contain poorly degraded organic compounds or not. As we worked on topsoil samples only, we consider that our samples contain poorly degraded organic compounds, as in Hazera et al. We will check both corrections (with or without considering that soil samples contain poorly degraded organic compounds) and comment on it in the revised version. Nevertheless, we consider that if the use of a correction method depends on something that is difficult for the user to determine, this means that such a method is unsuitable.*

To apply the Disnar's correction extended to Cinorg, Stojanova et al. (2024) propose using a threshold value of 2 gC/kg of SIC to determine which samples are calcareous or non-calcareous. However, the MinC parameter includes a portion of released Corg, particularly during the pyrolysis phase (Hazera et al., 2023; Koorneef et al., 2023). So, does the use of MinC to distinguish calcareous from non-calcareous soils introduce uncertainty in samples with high TOC? Since the comparison of models is conducted for three soil populations (non-calcareous, calcareous, all), have the authors verified the accuracy of these categories through mineralogical analyses (such as XRD) or through a detailed examination of thermograms (as in Pilot et al., 2014)? Another question concerns the minerals. Do the proposed models integrate soils containing minerals other than calcite? Thermograms of dolomite or siderite are quite distinct (Pilot et al., 2014). Could this impact the performance of the machine learning models?

*Answer : We thank the reviewer for this comment. We estimate that this would not make a significant difference, but there are indeed more appropriate ways of determining whether a soil sample is carbonated or not than the threshold we have chosen. The amount of C erroneously attributed to MinC comes mostly from the S3 and S3' signals (PyroMinC). We will determine if the sample is carbonated by comparing the OxiMinC and the PyroMinC. When OxiMinC is < 0.1 wt%, the soil sample can be regarded as non-carbonated whatever the PyroMinC values, which is organic carbon in that case.*

*From the thermograms, we determine that we don't have neither dolomite nor siderite. We will specify this in the revised version.*

One of the strengths of the work by Stojanova et al. (2024) lies in their explicit and unambiguous statement of the objectives of their approach: to identify the correction method that minimizes the discrepancies between the corrected RE measurements and the standard measurements used as reference. By correcting the RE measurements in this manner, the authors achieve a very satisfactory approximation to standardized measurements (ISO). This significant advancement will facilitate the practical use of RE data while awaiting their possible standardization. Concerning the comparison of models, the analysis is based on their respective performance in minimizing discrepancies with the reference method. However, the results are not analyzed relative to each other. Would it be possible to verify that the

differences between the methods are statistically significant considering the analytical precision of the methods used?

*Answer : Pairwise comparisons show that the differences between SOC and SIC values provided by the different methods are most often highly significant ( $p < 0.001$ ). In particular, outputs of the correction methods presented in Hazera et al. tend to overestimate SOC and are highly significantly different from those provided by the other correction methods. We will add some figures and paired T-test results on this aspect in the Notebook.*

However, minimizing the discrepancies between the corrected RE measurements and the standard measurements raises a more fundamental question: it is well-known that standard protocols for measuring SOC and SIC entail several inevitable errors related, on one hand, to sample pretreatment (removal of Corg or Cinorg), and on the other hand, to measurements on two different aliquots. Therefore, in seeking to minimize the discrepancies between RE measurements and the standard method, the authors import errors associated with the latter for calcareous soils. From a methodological perspective, it would be judicious to indicate this limitation in the technical note. Indeed, this inherent limitation to the stated objectives highlights the need for further studies to improve the initial measurement and correct the systematic misattribution of Corg as Cinorg.

*Answer : We will discuss this in the revised version. This is also the reason why we decided to have SOC and SIC measured in the French soil analysis laboratory . We are not sure that the « initial measurements » can be substantially improved.*

This is why the end of the abstract raises perplexity when the authors write: "that the proposed correction significantly increases the accuracy of the Rock-Eval method on the initial dataset, and that it can be successfully applied to data originating from different Rock-Eval machines, without changing the routine analytical protocol." This statement seems to be in contradiction with the objectives presented. The correction did not increase the accuracy of the RE method; it reduced the discrepancies of the measurements with a reference method that has its own errors. The RE method would increase its accuracy if the analytical protocol or calculation methods avoided confusion regarding the forms of carbon.

*Answer : In our view, the LAS provides the reference measurements, and so being able to supply SOC and SIC from Rock-Eval® data as close as possible to the LAS values corresponds to an increase in the accuracy of Rock-Eval measurements. However, we understand the subtlety of the reviewer's remark and will modify the sentence accordingly.*

In conclusion, one may question the format chosen by the authors to publish their results. Does the Technical Note format allow for the development of all the necessary discussions to truly highlight the results? This format, which minimizes the scientific issue in favor of the results, accentuates at the same time the "advertisement for the Rock-Eval device and Geoworks software" commercialized by the company that funded the study, both of which are used for commercial purposes by another party of the study's co-authors (which is not indicated in the section dedicated to potential conflicts of interest).

*Answer : We thank the reviewer for this remark, however we are not sure to fully understand what they mean by « the necessary discussions to truly highlight the results ». We think we have given a clear answer to a specific technical question that could greatly facilitate works in carbonate soils. Given the nature of the work itself, we think the Technical Note format is fully appropriate and encompasses the entirety of our contribution. The problem of carbon quantification in carbonated soils is a major one that severely limits the community's ability to study these soils. It is our shared belief that the work we present is far from an*

*advertisement for a machine and a software, and instead it represents a much-awaited solution for the scientific community. Moreover, we have made sure to make the data and routines freely available in an open-source language and platform, so any user can apply the proposed corrections without having to buy Geoworks.*