Responses to Reviewer 2

Please note that your comments are provided in green text and our responses are marked in blue text. Our major modifications in the revised manuscript are marked as red text.

The authors presented a new model to estimate soil bulk density and evaluate the performance using the LUCAS database. Overall, the manuscript was well written. The improved model performance will significantly help the research community to derive more reliable soil carbon stock products. I have some minor comments below:

Response: We would like to thank your positive feedbacks on our manuscript. We have replied your detailed comments one by one below. Hope you are satisfied with our revision.

1. In the two existing bulk density models, the input data is SOM. Please explain how you estimate this from the LUCAS data where the listed variables only have SOC. If you used a conversion factor to estimate SOM from SOC, can you please run some simple uncertainty analysis for the four existing models? For example, if you replace the SOM input in models #3 and #4 with SOC, you will get two new models that only use SOC as inputs. Then, a simple inter-model comparison can be made by plotting the estimated bulk density from four models vs. measured bulk density using a range of SOC inputs. However, if you used independent sources of SOM for models #3 and #4, some of the uncertainty may be attributed to analytical errors related to SOM and SOC measurements.

Response: Thank you for this remark. We fully admit that the conversion factor from SOC to SOM is a matter of discussion (Pribyl, 2010). However, we think that we should clarify the point about changing SOM by SOC in PTF-3 and PTF-

4. We used SOC to estimate SOM by multiplying SOC by the conventional coefficient of 1.724. We fully acknowledge that this coefficient is not universal (Pribyl, 2010). However, it remains the most used and we have no real indication that can tell us how we could modify it in a clever way. Therefore, the most important point is to ensure that the same conversion coefficients are used throughout the model comparisons. We go now more in depth to the points about PTF-3 and PTF-4.

PTF-3: The first use of PTF-3 is not from Sun et al. (2020), neither from Mann (1986) but from Adams (1973). In their study, Sun et al. (2020) indicated that they "converted SOC to SOM by dividing a coefficient of 0.58" (Mann, 1986) when the SOM is not given in the literature". This conversion coefficient has been used for nearly 2 centuries (Sprengel, 1826, cited by Pribyl, 2010). It corresponds to SOM=1.724×SOC and is often called the "van Bemmelen factor" (Van Bemmelen, 1890). In a critical review, Pribyl (2010) stated that this conversion factor could range from 1.4 to about 2.5, and suggested that 1.24 might be on average to low and that 1.9 or 2.0 might be preferable. All the studies involved in the meta-analysis from Sun et al. (2020) used published SOC or SOM data which are from cultivated soils (either conventional or conservation tillage). Though it is not clearly specified in the paper from Sun et al. (2020), neither in its supplementary materials, it is likely that most of the original data used by Sun et al. (2020) came from SOC measurements, which are most of the time used to derive SOM (and not the reverse), especially in cultivated soils. In other words, some papers from the meta-analysis of Sun et al. (2020) used SOM for reporting, though they actually used SOC to estimate SOM by the coefficient of 1.724. When they had only SOC, Sun et al. (2020) used conversion to SOM too, because they used the original PTF from Adams (1973), and refitted it using their data. The Adams' equation refers to SOM because its aim is to consider the relative % of organic and mineral compounds in soil as if they were independent (except for the fact that they sum to 100%).

It is the reason why, in the Adams' ratio, 100% is used as numerator and SOM% and (100-SOM%) are used in the denominator. We have good reasons think that this Adam's equation used in PTF-3 is conceptually wrong because it does not consider interactions between organic and mineral compounds, but it is the basic hypothesis from Adams. Note that Adams constructed this equation in podzolic soils in which most SOM is particular and not complexed with clay minerals, especially in topsoil horizons (Jolivet et al., 1998). Knowing this hypothesis and the Adams' formula, using SOC% to replace SOM% in the PTF-3, using the 100% as a reference for the whole soil does not make sense from a conceptual and physical point of view, because the total does no more sum up to 100%. Doing this would make the implicit hypothesis that SOM=SOC and that the Van Bemmelen factor is equal to 1. To check it, we replaced SOM by SOC as you suggested and came to a strong decrease of R^2 from 0.41 to 0.31.

PTF-4: On the contrary, the PTF-4 does not make the same hypothesis based on (mineral compounds + organic compounds) = 100%. It just modulates a constant value of BD using an exponential decreasing effect SOM. Tao et al. (2023) used SOC content. To convert them into SOC stocks, they "used a pedo-transfer function to estimate the bulk density.

BD = $\alpha + \beta \times \exp(-\gamma \times \text{OM})$

where OM is organic matter, calculated as SOC × 1.724".

Therefore, changing SOM by SOC does not change the fitting. Mathematically, using the equations

$$BD = a + b \times \exp(-c \times \%SOM)$$

or

$$BD = a + b \times \exp(-c \times \%SOC)$$

will result exactly in the same fitting, but with a change of the coefficient *c* which will be multiplied by 1.724 (or another value of the Van Bemmelen factor if we have a good reason to use this value). Therefore, in this case the R^2 remains the same and the predicted values of BD do not change, but, of course, the coefficient *c* of the equation changes. Thus, we have added relevant parts in the discussion in Lines 366-377: “We acknowledge that our uses of PTF-3 and PTF-4 are based on measured SOC contents and on a fixed Van Bemmelen factor (SOM=1.724×SOC, Sprengel, 1826; Van Bemmelen, 1890) to convert them into SOM. One good reason to use this factor is that it enables a comparison with most of the studies predicting BD using SOC and other soil properties. One pitfall is that we know that the conversion factor from SOC to SOM is not constant (Pribyl, 2010). First, we recall that we used this conversion factor for PTF-3 and PTF-4 only. Besides, considering the equations used, changing this conversion factor for PTF-4 has no consequence on the predicted absolute values of BD, neither on the goodness of the fit of the PTFs predicting BD. On the contrary, changing the conversion factor for PTF-3 will have consequences. We have no clear indication to try to adapt the Van Bemmelen factor to the pedological context (neither the effect of SOC on BD) when we use fixed regressions such as in PTF-1, PTF-2, PTF-3, and PTF-4. One advantage of ML-PTFs and especially of local ML-PTFs is that they can take into account interactions between soil properties. Therefore, the importance of SOC likely varies depending on other local controlling factors such as clay content or climate or even the nature of the organic compounds, which could explain the strong effect of N. In other words, ML-PTFs are able to partially compensate for the effect of using a fixed conversion factor between SOC and SOM.”

Apologises for this long reply to your suggestion. Hope you are satisfied with it.

References in the manuscript

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Van Bemmelen, J.M.: Über die Bestimmung des Wassers, des Humus, des

Schwefels, der in den colloïdalen Silikaten gebundenen Kieselsäure, des Mangans u. s. w. im Ackerboden Die Landwirthschaftlichen Versuchs-Stationen, 37, 279-290, 1890.

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2. Please explain a bit more about the depth of the soil samples. It seems that you only build the models and compare your models with other models for the depth of 0-20 cm. My question here is that your machine learning models share the same climate/terrain predictors but different soil property predictors. What

will happen if the authors want to estimate soil bulk density at a soil profile at different depths or even for 0-5 cm or 0-15 cm within the dataset you have? Will the coefficients stay the same for different depths? It may be helpful to publish another reduced model without climate/terrain predictors for an improved applicability/transferability of your more accurate models so that researchers can use them for bulk density estimation at different depths, just like the current models.

Response: Thanks for your simulating comments and suggestions. The LUCAS Soil only recorded soil information at 0-20 cm deep for the last three sampling campaigns (for the year of 2009, 2015 and 2018). Therefore, we have only generated all the PTFs for a depth at 0-20 cm and we are not able to generate a model applicable for deeper soil layers or upper ones (0-5 cm). However, we stress in the paper that this should be an objective for the future. This limitation has been mentioned in the discussion in Lines 358-363: "It is essential to acknowledge that our developed PTFs for BD_{fine} prediction was constructed based on LUCAS Soil data (0-20 cm), confining its applicability to topsoil within the EU and UK (Orgiazzi et al., 2022, Panagos et al., 2022). However, the potential of their extrapolation capability to other regions or to deep soil (>20 cm) necessitates further evaluation. As more soil data become available from diverse regions as well as for deep soil (Lal, 2018; Tautges et al., 2019; Batjes et al., 2020; Yost et al., 2020), the proposed methodology can be further used to update the PTFs, thereby broadening its area of applicability (Chen et al., 2018; Meyer and Pebesma, 2021).".

Of course, if people have access to depth-specific soil bulk density data, they can develop depth-explicit machine learning models to account for the effects of climate and terrain on bulk density at depths. However, I think the research community has not well studied this issue and it will be a very important topic for future collaboration.

Response: Your suggestion is quite simulating for future work. We share the same point of view that depth-explicit machine learning based PTFs would be important for more accurate estimate BD since it can account for the effects of climate and terrain on bulk density at depths. As you mentioned, depth-specific soil bulk density data along with depth-specific soil properties would be required to build such PTFs. This suggested has been added in Lines 363-365: "In addition, when a depth-specific soil BD_{fine} database is available, it will be important to develop depth-explicit ML-PTFs to account for the effects of climate and terrain on BD_{fine} at depths.". In summary, we fully agree with you that this will be a very important topic for future collaboration.