Reply to Anonymous Referee #1 for "Prediction of Peat Properties from Transmission Mid-Infrared Spectra"

Henning Teickner[1,2,*] Klaus-Holger Knorr[1]

10 January, 2026

[1] ILÖK, Ecohydrology & Biogeochemistry Group, Institute of Landscape Ecology, University of Münster, 48149, Germany
[2] IfGI, Spatiotemporal Modelling Lab, Institute for Geoinformatics, University of Münster, 48149, Germany

[*] Correspondence: Henning Teickner <henning.teickner@uni-muenster.de>

We thank the reviewer for the helpful comments and hope to have addressed them appropriately. Comments made by the reviewer start with a bold **Q** while our reply starts with a bold **A**. In section "Additional changes" we list additional changes we would like to incorporate in an updated version of the manuscript.

1 Reply to comments

1.1 Comments

1. **Q:** The introduction features repeated reference to Bulk density as a predictable property through spectra in mineral soils, on lines 54 and 69. This physical property is influenced in situ by landscape position, biotic interactions and soil composition. Many would not regard it as a property that is commonly considered predictable through spectroscopic approaches, particularly in cases where spectra are sampled in laboratory conditions, after soil processing. Though Dangal and Sanderman have modeled BD observations to moderate success with MIR spectra, other studies, such as Minasny et al 2008 suggest that properties that involve soil-pore relationships are less reliably predicted, which is logically consistent for analysis on disturbed soil.

   As this potential to model BD underpins the proposed pedotransfer functions for porosity, hydraulic conductivity, specific heat capacity and thermal conductivity, the paper requires more depth in the introduction on developments or suggestions that would argue against this thesis.

See: Minasny, B., McBratney, A. B., Tranter, G., & Murphy, B. W. (2008). Using soil knowledge for the evaluation of mid-infrared diffuse reflectance spectroscopy for predicting soil physical and mechanical properties. European Journal of Soil Science, 59(5), 960–971. https://doi.org/10.1111/j.1365-2389.2008.01058.

A: The comment refers to the fifth paragraph of our Introduction, where we give a brief overview on the potential of MIRS to predict various soil properties. The referenced lines give a couple of examples of soil properties that can be predicted from MIRS with some success, but we do not state that MIRS prediction models are an error free method. Our main intention here was to introduce MIRS prediction models as useful method to predict some soil properties.

We agree with the reviewer that it is important to understand why it should be possible (or should not be possible) to predict certain soil properties from mid-infrared spectra (MIRS) with a desired prediction error. We certainly also agree that one would expect that predictions of bulk density from MIRS have larger errors (relative to other soil properties) than properties that do only depend on the chemical composition (e.g., nitrogen content), because of the many factors that control bulk density but do not depend on the chemical composition of the soil particles.

While these points are important, we do not think that a more in-depth discussion of these issues fits within our manuscript. A discussion of these issues is from our point of view rather complex and may go beyond the scope of our manuscript. Quite a bit of text might be necessary to detail these points adequately. We think that a full discussion of all potential limitations may rather represent an own review article.

Referring to the bulk density debate, we do neither think that Minasny et al. (2008) contradicts the findings from Dangal et al. (2019), nor that Dangal et al. (2019) or our statement about this study exaggerate the potential of MIRS to predict bulk density (Dangal et al. (2019) states "For bulk density, which is a more difficult to predict soil property …").

Prediction errors in Dangal et al. (2019) and Minasny et al. (2008) are about equally large ($RMSE_{test}$ of 0.16 g cm^{-3} (Tab. 4 in Dangal et al. (2019)) and $RMSE_{test}$ of 0.09 g cm^{-3} (Tab. 4 in Minasny et al. (2008))). We assume that both papers came to contrasting conclusions merely because the range of bulk density values in Minasny et al. (2008) is much smaller than that in Dangal et al. (2019) and therefore relative prediction errors are larger in Minasny et al. (2008) than in Dangal et al. (2019). This is also ackowledged in Minasny et al. (2008) (Subsection "Bulk density" in section "Results and Discussion" in Minasny et al. (2008)). Wether or not prediction errors are small enough for predictions to be useful depends on the specific purpose of the analysis of the predictions and therefore can be argued in a general way only in rare cases where prediction errors are extremely large. We do not think that prediction errors are extremely large for the bulk density model from Dangal et al. (2019) or the model developed here.

Apart from this issue, the process of measuring bulk densities of mineral soils is not trivial and probably produces larger errors than other measurements (e.g., nitrogen content). One would therefore also have to discuss potential propagation of measurement errors into prediction errors of MIRS prediction models.

Since we focus on peat, we would also have to discuss how controls are different for organic soils, that have a known relation between bulk density and organic matter composition due to the dependence of structural integrity of peat on intact cell walls (e.g., Dykes, 2008). In addition, MIRS can distinguish well between organic matter and minerals and much of the bulk density gradient in peatlands is controlled by more minerals. All these points would have to be discussed, too.
Moreover, we do not think that it is always possible to anticipate whether a soil property can be predicted with some desired accuracy with MIRS or not because it is usually the case that prediction works because of correlations rather than causal controls and these correlations are not easy to anticipate. For example, MIRS can differentiate between quartz and clay minerals and both often have different particle sizes and hence lead to different porosities and therefore bulk densities (e.g., Minasny et al., 2008) and this probably is one reason why bulk density can be predicted from MIRS to some degree.
Finally, similar issues would also apply to other properties for which we computed models and and following the line of argument, we would have to discuss also here potential limitations. We think that this goes well beyond the scope of our study.
We therefore see it as our responsibility to provide users of our models with an as accurate estimate of prediction errors as possible (also models that combine the MIRS prediction model for bulk density with the pedotransfer functions do propagate prediction errors from the MIRS prediction model for bulk density) and let them decide whether these prediction errors are acceptable for their purpose or not.

2. **Q:** Similarly, isotope ratios of 13C and 15N are introduced following the aims of the paper as a property of interest to model. Given their under-performance, and general absence from modelling in other soil spectral libraries, a deeper dive into both the utility of this information, and justification for what about the variation in 13C and 15N ratios can be detected within the MIR region. If this is exploratory in nature, as indicated by the results, and the minimal gap filling achieved in pmird, it is important to temper the reader's expectations here appropriately.

   A: We thank the reviewer for this suggestion. While the abstract already mentions that prediction errors are large for δ^{13}C and δ^{15}N, we agree that it is useful to mention this result also in the Introduction. To this end, we changed the sentence in l. 123 to 124 from:

   "While some of our models may only generate approximate predictions, many have prediction errors small enough to be useful in diverse applications."

   to:

   "While some of our models may only generate approximate predictions (especially δ^{13}C and δ^{15}N), many have prediction errors small enough to be useful in diverse applications."

3. **Q:** The prediction domain of the models generated from pmird is highly dependent on

the observed variation in peat analytical data and spectra available in the database. A sound understanding of the model calibration space is important to reduce mis-application of the models. As such, some greater exploratory data analysis on the pmird data can provide additional context to the reader, perhaps a table of summary statistics of the properties to be modelled, and the map showing the distribution of peat samples that comprise this dataset. As the pmird database itself is in pre-print, this does not need to be extensive here.

A: We agree with the reviewer that it is important to avoid mis-uses of MIRS prediction models. In fact, we computed the prediction domains with the intention to avoid application of models to inappropriate samples. However, we think that our manuscript either already provides the information requested by the reviewer or that suggestions of the reviewer do not add more than the prediction domains already provide.
Tab. 2 provides the value range for each variable. While we could add more summary statistics, we do not think that this would be useful to avoid mis-application of the models because extrapolation errors depend directly on the spectral properties and only indirectly on other peat properties or where peat samples were taken. We therefore think that the prediction domains are sufficient for a first check whether the models may be applicable, detect more errors (for example differences in baseline correction) than would be possible from the suggested summary statistics or a map of peat sampling loations, and are implemented in 'irpeat' and therefore easy to apply.
We welcome in-depth analyses and ciriticism of our models and in this case, all data are available from the pmird database (Teickner et al., 2025) and the R code we published (Teickner and Knorr, 2025) and we think scientists who want to criticize/improve our models would rather consider these resources than additional summary statistics.
To avoid mis-interpretation of prediction domains as error-free check, we suggest to add the following sentence after l. 255 (old, new: l. 257 to 260): "This test of MIRS against prediction domains is only a first test because even spectra within the prediction domain may have spectral properties and values for the predicted peat property that are different from the training or test data. With a large enough training and test dataset, such edge cases become more and more unlikely. Additional checks to be provided by future studies are based on a list of error sources identified through targeted tests of the models against such possible edge cases."

4. **Q:** The presented model quality metrics are an important consideration that guide potential users and readers to a greater understanding of the implications of your work. As such, if the work adapts techniques from spectral modelling of mineral soils, It could benefit the ease of interpretation of the work to further adapt some commonly used quality metrics as well. I would suggest initially the MEC, RPIQ and LCCC as useful guides that users more familiar with modelling of mineral soils may useful.

   See: Bellon-Maurel, V., Fernandez-Ahumada, E., Palagos, B., Roger, J.-M., & McBratney, A. (2010). Critical review of chemometric indicators commonly used for assessing the quality of the prediction of soil attributes by NIR spectroscopy. TrAC Trends in Analytical Chemistry, 29(9), 1073–1081. https://doi.org/10.1016/j.trac.2010.05.006

   A: We thank the reviewer for this suggestion. Studies on models for mineral soils also

regularly use the quality metrics presented here in Tab. 2, in particular $\mathrm{RMSE}_{\mathrm{test}}$ (= RMSEP = SEP in Bellon-Maurel et al. (2010)) and bias. Thus, the results presented in Tab. 2 should be understandable and useful also for users more familiar with modelling of mineral soils.
While we agree that MEC, RPIQ and LCCC provide different summaries than $\mathrm{RMSE}_{\mathrm{test}}$ and bias, we do not think that these metrics are particularly useful, mainly because they do not summarize predictive performance on an absolute scale (in native measurement units) and therefore deliberately omitted them:

1. MEC is defined as $1 - \frac{\mathrm{RMSE}_{\mathrm{test}}}{\sigma}$, where σ is the standard deviation of the data. It is therefore an estimate for the variability of the data that can be explained by the model. A similar metric is RPD which is defined as $\frac{\sigma}{\mathrm{RMSE}_{\mathrm{test}}} = \frac{1}{1-MEC}$ and therfore is simply MEC expressed differently. MEC and RPD depend on both the standard deviation of the training data and prediction errors and therefore mix predictive accuracy with the representativenes of the data (assuming that datasets with larger standard deviation are more representative overall beause they are apparently mor diverse). For example, MEC does not distinguish between a model that predicts the C content with an error of 0.02 g/g and trained on data where the C content has a standard deviation of 0.1 g/g and a model that predicts the C content with an error of 0.1 g/g and has a standard deviation of 0.5 g/g. We think both cases should be separated and we think that users of a model would rather like to know how well a peat property can be predicted on an absolute scale.
2. RPIQ is similar to RPD, but replaces σ by the interquartile range. This makes the metric more robust against non-normality, but it still measures a ratio of prediction error to training data variability and therefore mixes both properties.
3. LCCC detects deviations of pedictions from the data caused by bias or spread and is therefore useful as a one-number summary of the reproducibility of measurements (Lin, 1989). Bias, $\mathrm{RMSE}_{\mathrm{test}}$, and the plots of measured versus fitted values provide similar information.

Therefore, we prefer to provide fewer but more relevant/equivalent metrics that can be interpreted on the scale of measurement of the peat properties of interest.

1.2 Additional clarity issues

5. **Q:** Lines 33–38: The paragraph is vague regarding "sufficient resolution and detail." Define what constitutes "sufficient."

   A: Unfortunately, we are not able to locate the quote "sufficient resolution and detail" in our manuscript. Perhaps the reviewer refers to "… quantify global peat properties at sufficient spatial resolution …" (old: l. 34) from the referenced paragraph?
   "sufficient spatial resolution" means here a spatial resolution high enough for the different use cases of peat data mentioned in the previous paragraph is achieved. For

example, errors in stock estimates caused by the large spatial variability of peat properties could be decreased if such data were available at higher spatial resolution. While it is not clear how large these errors are, often only one central peat core pear peatland is sampled and spatial variabilities in the concentration of compounds, for example C, are not considered in stock calculations (e.g., Loisel et al., 2017).

To avoid misunderstandings, we suggest to replace:

"… quantify global peat properties at sufficient spatial resolution …"

by

"… quantify global peat properties at high spatial resolution …"

6. **Q:** Lines 233:236: Sentence is quite long, with many clauses, please break this up.

   A: We thank the reviewer for this suggestion. While the referenced sentence is long, it has the simple structure of a list of clauses starting with "because" and justifying why we do not interpret model coefficients; therefore, we do not think that it is too complicated, and we prefer to keep all justifications in one compact list. To facilitate reading, we added an enumeration (new: l. 234 to 237):

   "We do not interpret model coefficients and how this may reflect causal links between molecular structures and target variables (1) because our model coefficients are not intended to estimate causal effects, (2) because it is very likely that they do not represent causal effects, and (3) because specific wavenumbers cannot be assigned unambiguously to molecular structures (e.g., Stuart, 2004)."

7. **Q:** Line 240: this paragraph repeats context established in the introduction, much of this is redundant within the methods.

   A: While we agree that this text is partly redundant, we prefer to keep this redundancy because the concept of using a prediction domain for spectral prediction models is new for potential users of spectral prediction models for peat who have no overview on the modeling literature for mineral soils and because we have the impression that many researchers who use spectral prediction models for peat are not aware of the importance of checking extrapolation by the models.

8. **Q:** Lines 377:385: The discussion on blank effect corrections for isotopic measurements is confusing. It first suggests these effects are only a minor contributor to RMSE, then proposes they may explain large prediction errors. This whole argument is quite confusing, consider omitting lines 384/385 for clarity.

   A: We thank the reviewer for this suggestion. We omitted lines 384 zo 385, as suggested.

9. **Q:** In figure 4, fixing the y axis, and grouping the facets by derivative of spectra may make the prediction domains easier to interpret across the different properties being assessed.

   A: We thank the reviewer for this suggestion and we agree that it is useful to be able to compare the prediction domains between variables. To do so, we decided that for

the plot, we preprocess the spectra and scale the intensities in the same way across all target variables so that the prediction domain for a variable can be directly compared to that of any other variable. We updated the figure accordingly.

2 Additional changes

1. old: l. 379 to 380; new: l. 385 to 386: We moved the ‰ sign in front of the parentheses.

2. old: l. 308; new: l. 313: We added "(e.g., Bellon-Maurel et al., 2010)" as a new citation to point to the relevant discussion about the comparability of prediction errors in Bellon-Maurel et al. (2010).

References

Bellon-Maurel, V., Fernandez-Ahumada, E., Palagos, B., Roger, J.-M., and McBratney, A.: Critical review of chemometric indicators commonly used for assessing the quality of the prediction of soil attributes by NIR spectroscopy, TrAC Trends in Analytical Chemistry, 29, 1073–1081, https://doi.org/10.1016/j.trac.2010.05.006, 2010.

Dangal, S., Sanderman, J., Wills, S., and Ramirez-Lopez, L.: Accurate and precise prediction of soil properties from a large mid-infrared spectral library, Soil Systems, 3, 11, https://doi.org/10.3390/soilsystems3010011, 2019.

Dykes, A. P.: Tensile strength of peat: Laboratory measurement and role in Irish blanket bog failures, Landslides, 5, 417–429, https://doi.org/10.1007/s10346-008-0136-1, 2008.

Lin, L. I.-K.: A concordance correlation coefficient to evaluate reproducibility, Biometrics, 45, 255, https://doi.org/10.2307/2532051, 1989.

Loisel, J., van Bellen, S., Pelletier, L., Talbot, J., Hugelius, G., Karran, D., Yu, Z., Nichols, J., and Holmquist, J.: Insights and issues with estimating northern peatland carbon stocks and fluxes since the Last Glacial Maximum, Earth-Science Reviews, 165, 59–80, https://doi.org/10.1016/j.earscirev.2016.12.001, 2017.

Minasny, B., McBratney, A. B., Tranter, G., and Murphy, B. W.: Using soil knowledge for the evaluation of mid-infrared diffuse reflectance spectroscopy for predicting soil physical and mechanical properties, European Journal of Soil Science, 59, 960–971, https://doi.org/10.1111/j.1365-2389.2008.01058.x, 2008.

Stuart, B. H.: Infrared spectroscopy: Fundamentals and applications, John Wiley & Sons, Ltd, Chichester, UK, https://doi.org/10.1002/0470011149, 2004.

Teickner, H. and Knorr, K.-H.: Compendium of R code and data for "Prediction of Peat Properties from Transmission Mid-Infrared Spectra", https://doi.org/10.5281/ZENODO.17209177, 2025.

Teickner, H., Agethen, S., Berger, S., Boelsen, R. I., Borken, W., Bragazza, L., Broder, T., De La Cruz, F. B., Diaconu, A.-C., Dise, N. B., Drollinger, S., Estop-Aragonés, C., Gałka, M., Martí, M., Glatzel, S., Groß, J., Harris, L., Heffernan, L., Hodgkins, S. B., Hömberg-Grandjean, A., Hoppe, H., Kleinebecker, T., Knierzinger, W., Liu, H., Mathijssen, P. J. H., Mollmann, C., Schuster, W., Närtker, L., Olefeldt, D., Pancotto, V., Pelletier, N., Reuter,

H., Robroek, B., Svensson, B., Talbot, J., Thompson, L., Worrall, F., Yu, Z.-G., and Knorr, K.-H.: Peatland mid-infrared database (1.0.0), https://doi.org/10.5281/zenodo.17092587, 2025.