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Comment on soil-2022-27

Anonymous Referee #1

Referee comment on "Improving models to predict holocellulose and Klason lignin contents for peat soil organic matter with mid-infrared spectra" by Henning Teickner and Klaus-Holger Knorr, SOIL Discuss., https://doi.org/10.5194/soil-2022-27-RC1, 2022

This is an excellent manuscript based on an excellent rationale with sound research questions. It is very well structured and very well written. Building on previous data and models, Teickner & Knorr provide detailed explanations of the steps followed to evaluate the models, describing the limitations (representative of the training data sets, validation of the models, availability of key data of the models' output, biases and uncertainties, etc.) and potential improvements. This research also shows the key importance of a detailed analysis of the models' residuals as a way to identify model's deficiencies. It is also a key finding that OM composition of mineral soils can also be accurately modeled. This research also shows the potential of MIR for SOM characterization and modelling and the importance of making data and code available for further improvements.

Regarding the general issue of the preselection of peaks before modelling, one possible alternative is to perform PCA on all detected peaks to reduce the dimension and extract the most relevant spectral signals. PCA is usually efficient in allocating into different components the overlapping effects of more than one compound on a given spectral band/region.

Specific comments

L277-279. Positive and negative coefficients for peaks at 1150 and 1270 cm-1 (aromatic C-H bending). This may be due to they reflecting different lignin structures: 1270 cm-1 surely corresponds to guaiacol (G) moieties and 1150 cm-1 could correspond to syringol (S) moieties (although S most representative band is at 1310 cm-1). Both differ in content in the source peat vegetation and also show differences in resistance to degradation in peat depending on oxygen availability (see for example, Schellekens et al. 2012 Soil Biology and Biochemistry 53, 32-42). G lignin is less prone to degradation than S lignin and the G/S ratio of fen peat (more decomposed) is larger than that of bog peat (less decomposed) (see for example Martínez Cortizas et al., 2021 Boreas 50, 1161-1178).

L380. I agree. Due to overlapping of spectral absorbances some peaks are contributed by more than one peat component. We have found quite similar results for modelling C and N content in peat (ongoing): residuals of aromatic and protein vibrations are highly correlated to C and N models' residuals, and their inclusion in the models results in significant improvements in prediction. Thus, this effect seems to also have implications for modeling C and N content in peat a long-term scale and, thus, to evaluate the effects Holocene environmental change.

L.424 I find this "implication" to be quite important and other ways of spectral normalization should be tested in the future