Reply to Anonymous Referee #1 for "Estimation of the Degree of Decomposition of Peat and Past Net Primary Production from Mid-Infrared Spectra"

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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:** However, given the current limitations, these should be more clearly highlighted in both the title and the abstract, for example by framing the study explicitly as a "first step" or "proof-of-concept."

   A: We agree with the reviewer that we did not address all limitations of the suggested method and there will probably remain limitations that cannot be addressed at all. While we provide a detailed description of limitations in the Discussion section and the last sentences of the abstract (old: l. 15 to 18) point to limitations of the method

and steps that are necessary to improve it, we hope to avoid confusion by emphasizing even more in the abstract that the method still has limitations and requires further validation. To this end, we suggest to add at l. 15 (old, new: l. 15):

"The method requires further validation by future studies."

We think that any new method that has not been validated under circumstances where it might be applied should be considered as proof-of-concept, including the suggested method to estimate γ from MIRS. We do not think that our title implies that the method has no flaws, and we think that the title of the manuscript is already quite long. In addition, while we agree with the reviewer that our method needs further validation (and thus is a proof-of-concept), in the context of decompostion indicators and estimating the degree of decomposition of peat, the suggested method is certainly among the better tested methods: Firstly, qualitative decomposition indicators are, to our knowledge, not as well tested against measurements of γ from as diverse litter samples as used here. Reviews of decomposition indicators focus on comparing different decomposition indicators, but not on testing decomposition indicators with measurements from litterbag experiments (e.g., Biester et al., 2014; Zaccone et al., 2018). Secondly, the bias due to mixing litter types of different degree of decomposition is not mentioned in manuscripts suggesting or using decomposition indicators that may be considered as established. Explicit labeling our method as proof-of-concept might therefore be misunderstood by peatland researchers. We therefore prefer not to extent the title of our manuscript.

2. **Q:** In addition, it should be emphasized in the abstract, discussion, and conclusions that this method alone does not yet appear sufficiently robust to be applied independently, and that it should be used in combination with more established palaeo-reconstruction approaches (e.g. macrofossil analysis). The use of this approach for other research will demonstrate its usefulness and accuracy in the future.

   A: The study provides some tests of the suggested method (sectios 2.4 and 2.5) and the Discussion provides, based on these tests, a list of the limitations of the suggested method (sections 4.1 and 4.2). These limitations are also mentioned in the abstract (old: l. 15 to 18) and the conclusions (old: l. 610 to 615). We therefore do not think that any further emphasis of the limitations is necessary.
   While we agree with the reviewer that the method needs further validation (see also our reply to comment 1 of reviewer 1), we do not think that it is useful to use "more established palaeo-reconstruction approaches (e.g. macrofossil analysis)" in combination with the suggested method to somehow account for a potential lack of robustness of the method, as the reviewer seems to suggest. We think that the only sensible way to test the approach is to conduct tests with more diverse litterbag data (more diverse in terms of species, organs, and decomposition conditions), as suggested in our manuscript. Comparison to peat core data does not help because the degree of decomposition of peat cannot be measured directly, to our knoweldge, except with the suggested method.
   We might misunderstand the reviewer here. If the reviewer disagrees with our view, it would be helpful if the reviewer would more explicitly describe his suggestion and

how this would validate estimates for γ. In particular, the following points were not entirely clear to us:

1. We do not understand what "established palaeo-reconstruction approaches" are. The reviewer mentions "macrofossil analysis" as only example. We already suggest to use macrofossil analysis (ideally with estimates of mass fractions arrived at with a well tested method instead of volume fractions) to estimate the degree of decomposition of peat (e.g., old: l. 96 to 110 (Introduction), sections 2.6 and 4.1).
2. We do not understand in which way using "established palaeo-reconstruction approaches" would help. For example, other than the application of macrofossil analysis results described in the previous paragraph, we do not see how macrofossil analysis results should somehow account for a potential lack of robustness of the suggested method, given that macrofossil analysis does not measure the degree of decomposition and that macrofossil analysis is not sufficiently validated (e.g., Belyea, 2007; Väliranta et al., 2007).
3. The reviewer may have had in mind that established decomposition indicators — such as carbon to nitrogen ratio (C/N), humification indices, or oxygen to carbon ratio (O/C) (e.g., Biester et al., 2014; Zaccone et al., 2018) — could somehow account for a potential lack of robustness of the suggested method. However, as pointed out in the Introduction (old: l. 47 to 56), established decomposition indicators are not well tested and have many limitations (some of which are addressed by the suggested method). It does therefore not seem useful to use established decomposition indicators to somehow account for a potential lack of robustness of the suggested method.

3. **Q:** I strongly suggest including a schematic or conceptual figure that clearly explains the overall modeling workflow, from the training samples to the final results, including the different tests performed. Such a figure should indicate at which stages MIR analyses are conducted, as well as the input and output data at each step. This would greatly improve the clarity of the methodological approach for the reader.

   A: We thank the reviewer for this suggestion. We included a new Fig. 1 that shows the two possible workflows to estimate γ (either from bulk MIRS measurements and macrofossil volume fractions, using the mixing model, or from component-specific MIRS measurements and the masses of individual components) and referenced it in the main text where appropriate.
   We do not think that figures for the creation of the prediction models or their validation would be very useful because these figures would either abstract too much or get visually quite complex (if more detail is included). If the reviewer has concrete suggestions for how such figures should look, we would be glad to consider these suggestions.

4. **Q:** The description of the methods could also be improved. For example, the main text should provide more detailed information on the litter-bag experiments used in the training dataset, including the number of samples, incubation durations, and the specific time points at which samples were analyzed by MIR.

A: We suggest to add these information at l. 137 to 140 (old; new: l. 138 to 143):

"For our analyses, we used the following litterbag data: *Sphagnum capillifolium* (capitulum and first 5 cm of the stem; 20 samples) and *Typha latifolia* (leaves; 20 samples) samples incubated in bog peat and pools (oxic and anoxic conditions) in Canada for 808 days (Arsenault et al., 2024a, b), and *Phragmites australis* (leaves and rhizomes; 36 samples) grown under different nutrient availability and incubated under anoxic conditions in peat with different nutrient availability for 75 days (Reuter et al., 2019b, a; 2020). In both cases, MIRS were measured for the undecomposed litter and at the end of the incubation period."

5. **Q:** In addition, the manuscript frequently refers to previous studies by the authors, with which readers may not be familiar. I recommend providing more explicit descriptions rather than assuming prior knowledge — for instance, clearly explaining what the pmird database is and whether the MIR data from the peat cores are included within this framework.

   A: We thank the reviewer for this suggestion. We replaced the acronym "pmird" by the full name "Peatland Mid-Infrared Database" to provide a more explicit description. The text already mentions (old: l. 157 to 158) that the peat core data are derived from the Peatland Mid-Infrared Database ("… we used bog peat core measurements derived from the pmird database …").

6. **Q:** Did the authors take any measures to check whether there were any differences between the instruments used to measure the MIR? Quality control?

   A: The MIRS in the Peatland Mid-Infrared Database are compiled from previous studies where MIRS were measured on different devices (see also section 2.1 in the main text). It is therefore possible that some differences between the spectra were also caused by differences in sample preprocessing and measurement devices. We are aware that this is a potential problem and therefore explicitly mentioned that different measurement devices were used. The preprocessing steps performed here are assumed or have shown to reduce differences between devices (e.g., Safanelli et al., 2023), but we have no information to check whether different devices may have caused some artefacts. The fact that γ can be predicted well for diverse litter samples with MIRS measured on different devices indicates that these artefacts are rather small compared to other error sources (this observation is of course only an indication and not a thorough test). We do not think that it is currently realistic to measure a similarly large dataset of litter samples and litterbag samples on one specific device. Therefore, the best way to test the influence of such factors is to test our models with new litterbag experiments where MIRS were measured on different devices.
   To our knowledge, differences in spectra between devices are poorly understood and the problem of transfering prediction models between devices (calibration transfer) is an open problem (e.g., Workman, 2018; Safanelli et al., 2023). Since we do not have specific information to add (none of the samples was measured on all the specific devices with the same settings), we did not discuss this problem in detail.

7. **Q:** With respect to nitrogen content, it would be helpful to explicitly state how many samples have measured nitrogen concentrations and how many values are predicted.

   A: We thank the reviewer for this suggestion. Of the 169 samples, 17 had no N measurements. This information is now added at l. 225 (old; new: l. 228).

8. **Q:** The authors could also discuss the implications of this "double modeling" approach, in which nitrogen is first predicted and then used for comparison with degree of decomposition estimates that are themselves derived from MIR data.

   A: We do not see any problem in predicting both N and γ from the same MIRS, as long as the error properties of both predictions for the specific samples are well understood. MIRS allow prediction of peat N contents with comparatively small errors (Teickner and Knorr, 2026) and, as mentioned in our reply to comment 7 by reviewer 1, N contents had to be predicted only for a small fraction of samples. Moreover, for samples where Fig. 3 (former Fig. 2) has larger residuals and where we observed relevant patterns in residuals versus N contents, all N contents are measured.

9. **Q:** Peat samples represent a complex mixture of organic matter derived from vegetation at different stages of decomposition, as well as microbial biomass. This complexity can influence the molecular signals measured in peat, as classically demonstrated by Chapman et al. (2001). This point may be relevant to address more explicitly in the discussion, as some MIR bands measured in peat samples may partly reflect microbial-derived signals rather than plant-derived organic matter alone.

   A: We agree that during decomposition some of the plant organic matter is transformed to microbial organic matter and this matter contributes to the absorbance of mid infrared radiation at specific wavenumbers. We did not explicitly mention microbial compounds when describing peat as mixture of different litter types in the Introduction because it is generally assumed that microbial biomass contributes only small mass fractions to samples of northern peat (this is also mentioned on p. 1200 in Chapman et al. (2001) which was referenced by the reviewer) and therefore also contributes only relatively little to infrared absorption. In line with the studies that interpreted peat MIRS (e.g., Chapman et al., 2001; Cocozza et al., 2003; Tfaily et al., 2014), we therefore assume that microbial-derived signals play a minor role. Reuter et al. (2020) argue convincibly that bands around 1200 cm^{-1} in the litter MIRS analyzed here stem from microbial DNA, but they need to compute second derivative difference spectra to the undecomposed sample to detect such a signal, supporting our assumption that microbial biomass does not contribute much to the MIRS signal.
   Microbial biomass and necromass may have larger fractions in more decomposed peat and we assume that this would be primarily identified as "unidentifable organic matter" in a macrofossil analysis. Due to the lack of studies that explicitly identify bands dominated by microbial-derived compounds in northern peatlands, we do not like to discuss this issue in more detail. However, we agree with the reviewer that it might be useful to mention contributions of microbial-derived compounds in our text. We therefore suggest to change l. 74 to 75 (old) from:

"litter of different plant species and organs, possibly with different degree of decomposition and different changes of chemical components (e.g., cellulose, lignin, lipids) during decomposition, and minerals."

to (new: l. 75 to 77):

"litter of different plant species and organs, possibly with different degree of decomposition and different changes of chemical components (e.g., cellulose, lignin, lipids) during decomposition, microbial bio- and necromass, and minerals."

10. **Q:** It is somewhat surprising that no evaluation or comparison between the obtained degradation index and the C/N ratio is presented, despite the C/N ratio being widely used as an indicator of mass loss in peatlands and being relatively easy to measure. I suggest that the authors include such a comparison, as it could be particularly useful when evaluating model results and for further studies, at least for those peat cores where C/N ratios are available.

    A: We omitted such a comparison intentionally since we wanted to focus on the validation of the suggested method to estimate γ. However, we agree with the reviewer that it is useful to at least briefly show a comparison what could be inferred from C/N ratios if they were used to estimate γ.
    In contrast to the reviewer, we do not think that it is useful to compare γ predicted from MIRS to C/N for the available peat core data because for these samples, γ is unknown. It is therefore more useful to compare both γ predicted from MIRS and C/N to γ as observed in the litterbag samples. We have added a supporting figure that plots C/N versus γ as observed in the litterbag samples (Fig. S13). This plot shows that the relation between γ and C/N differs by litter type and therefore a direct relation between γ and C/N (in absolute terms) does not exist for the considered litter types; one would have to condition on litter type. For the comparison of γ predicted from MIRS versus γ as observed in the litterbag samples, the same plot is already contained in the first column of Fig. 2 in the main text.
    A similar comparison could be made with different humification indices (HI) that are also often used as qualitative decomposition indicator and can be computed from MIRS (e.g., Broder et al., 2012). Different HI are usually correlated (e.g., Broder et al., 2012) and we therefore added a second panel to the new supporting figure only for $HI_{1630/1090}$. Here, a similar pattern as for C/N is observable, probably because the intensity at 1630 cm^{-1} is largely controlled by N content which is different for different litter types and has different dynamics during decomposition depending on the litter type (e.g., Reuter et al., 2020).
    The new figure is referenced in the main text at l. 468 (old; new: l. 483):

    "The carbon to nitrogen ratio (C/N) and a humification index ($HI_{1630/1090}$) often used as decomposition indicators (e.g., Biester et al., 2014) have more variable relations to the measured γ for the same litter types (compare supporting Fig. S13 to Fig. 2)."

11. **Q:** In the discussion, I also miss a more quantitative treatment of models "over- or underestimation". Including percentages or value ranges would strengthen the discussion and allow a clearer assessment of model performance.

A: We think that "a more quantitative treatment of models "over- or underestimation". Including percentages or value ranges" should be placed in the Results section, as is the case (sections 3.1, 3.3, 3.4), and not (necessarily) in the Discussion section. Since requirements for the predictive accuracy of a method are defined by the project that applies the method and since we are not aware of alternative approaches to estimate γ of peat, we do not think that there is much to discuss here. We think that both the text and the models available from the 'irpeatmodels' package provide enough information for users of the models to judge their prediction errors under different conditions.

12. **Q:** There are some issues with the references that should be addressed. Two references appear with the same authors ("Teickner, H. and Knorr, K.-H.") but different titles, and a similar issue occurs for "Teickner, H., Pebesma, E., and Knorr, K.-H." Please ensure that each in-text citation can be unambiguously linked to a single reference in the bibliography. One of these references is a preprint, which should be considered carefully in the context of the publication process.

    A: Unfortunately, it is not clear what references the reviewer refers to and what issue the reviewer wants to point out:

    1. There are two references with authors Teickner, H. and Knorr, K.-H. (old: l. 799 to 802) and they have, of course, different titles since they are different references. These references were published in different years and are cited as "Teickner and Knorr (2022)" and "Teickner and Knorr (2025)". We do not see that there is an error here.
    2. Likewise, there are two references with authors Teickner, H., Pebesma, E., and Knorr, K.-H. (old: l. 810 to 814) and they have, of course, different titles since they are different references. These references were published in the same year (2025) and are cited as " Teickner et al. (2025c)" and Teickner et al. (2025), so there is no ambiguity here, either.

13. **Q:** Finally, I recommend rephrasing the end of Section 3.8. The text is somewhat wordy, and the long parenthetical sentences disrupt the reading flow.

    A: We thank the reviewer for this suggestion. We removed the parentheses from the last parenthetical sentence.

2 Additional changes

1. At l. 525 (old; new: l. 540 to 544), we suggest to add:

    "While not considered here, an additional limitation of the current litterbag data may be that they do not consider how litter preprocessing may bias mass losses from decomposition compared to decomposition under more natural conditions (e.g., Bärlocher, 1997; Teickner et al., 2025). This may confound relations between MIRS and γ under more natural conditions when making predictions with models trained on litterbag data. However, at the moment, it is not clear how serious this problem is."

Initially, we did not want to mention this issue because we do not address it in the study here and we did not want to complicate matters more than necessary. However, in hindsight, we think that it is useful to at least mention this possible limitation since it may also be relevant for studies that want to test or improve our models.

2. We replaced Teickner and Knorr (2025) by Teickner and Knorr (2026) which is the final published version of the same reference (a preprint).

3. We corrected typos in the names of some taxa.

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