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Estimation of the Degree of Decomposition of Peat and Past Net Primary Production from Mid-Infrared Spectra

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Abstract. The degree of decomposition of peat (γ) is useful to understand peatland degradation and peat accumulation, to reconstruct past net primary production (NPP), and to improve peatland models. None of the available decomposition indicators allows to estimate γ with sufficient accuracy. We suggest prediction of γ measured in litterbag experiments from mid-infrared spectra (MIRS) as a novel decomposition indicator, γ_{MIRS}, and compute prediction models for γ_{MIRS} with available litterbag experiments and litter data from diverse species from the Peatland Mid-Infrared Database. For individual litter samples, the prediction models fit the data well, have reasonable prediction errors (average RMSE between 0.09 and 0.12 g g^{-1}), and neither confound differences in litter chemistry nor differences in silicate contents with decomposition losses. We show that an underestimation of γ by γ_{MIRS} matches theoretical expectations; it can therefore be compensated, using plant macrofossil analysis data as a first approximation to mass fractions of peat components and a simple mixing model, or it can be avoided with component-specific measurements instead of bulk measurements. This allows to estimate γ of peat samples and of dominant litter types and therefore also to reconstruct past NPP. To illustrate the approach, we analyze three cores from European mountain bogs and discuss how it can be used to improve process models and support restoration of peatlands. In particular, we test previously suggested relations between the saturated hydraulic conductivity and γ, illustrate how γ measured on individual litter types may allow to use peat cores as natural litterbag experiments, and define reference states for γ and NPP for the three analyzed peat cores. Improvements to reduce prediction errors of the approach require more diverse litterbag data, especially woody species and more decomposed litter. Further improvements can be achieved with measurements of MIRS on individual macrofossil types instead of bulk measurements, and an improved estimation of mass fractions of macrofossil types in peat samples instead of assuming that macrofossil abundances equal macrofossil masses.

1 Introduction

Peatland mass and carbon balance are the difference of net primary production (NPP) as mass input and of decomposition as mass output. Theory and modeling studies suggest a complex feedback between decomposition and net peat accumulation (Bauer, 2004; Belyea and Baird, 2006; Morris et al., 2011; Waddington et al., 2015; Mahdiyasa et al., 2022). As a direct effect,

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decomposition decreases net peat accumulation because mass is lost from the system, but as an indirect effect, this mass loss decreases peat height, porosity, and hydraulic conductivity, which can increase surface wetness and therefore may increase litter production and decrease decomposition over longer time periods. Under some conditions, more decomposition can therefore increase future net peat accumulation (e.g., Quillet et al., 2013). Therefore, if we could accurately describe how decomposition is controlled by environmental conditions, we could improve both reconstructions of past and predictions of future peatland dynamics.

When analyzing peat accumulation and decomposition processes, an important quantity is the degree of decomposition (γ), the fraction of initial mass that was lost due to decomposition. It is directly measured in litterbag experiments and allows to estimate decomposition rates and how they are controlled by environmental conditions. Peatland models use these estimates to simulate decomposition in peatlands for decades to millenia (e.g., Frolking et al., 2010). However, litterbag experiments only cover short time periods which leads to imprecise estimates for parameters that take effect only over longer time periods, such as the slow-down of decomposition due to increasing recalcitrance of the material left behind (Frolking et al., 2001). The degree of decomposition is also used to estimate mechanical and hydrological properties that control the ecohydrological feedback, such as the Young's modulus (Mahdiyasa et al., 2022, 2023), bulk density (Frolking et al., 2010), and saturated hydraulic conductivity (Frolking et al., 2010; Morris et al., 2011, 2015a), but these relations have only been tested against qualitative decomposition indicators (Dykes, 2008; Morris et al., 2015a), if at all. Estimates for γ of peat are also useful to disentangle peat accumulation scenarios: an unfortunate consequence of the ecohydrological feedback is that both shallow and deep water table levels may lead to very similar peat heights and masses, two variables often used to test peatland models, but litter production, decomposition losses, the net mass balance, and the degree of decomposition differ between these contrasting scenarios (Ramirez et al., 2023). For this reason, estimates of γ for peat samples would be useful to distinguish between these scenarios and to obtain more accurate estimates for processes rates (Ramirez et al., 2023). Finally, if γ is known for a peat sample, one can directly estimate the initial mass of the sample as $m/(1-\gamma)$, where m is the final mass of the sample. The NPP can be computed from the initial mass if the peat core is dated and roots are not dominant in peat formation. Thus, γ is a central quantity when estimating parameters and reconstructing process rates.

It is currently not possible to measure γ for peat samples. Direct measurements of γ are currently only possible in litterbag experiments. For peat, several measurable properties (decomposition indicators) have been suggested to estimate differences in γ. Currently, only the ash residue method (e.g., Leifeld et al., 2011b, a) allows to estimate γ on an absolute scale, but this method has large errors (Krüger et al., 2016) and indirectly presupposes that one already knows the initial mass of a sample (we abbreviate γ estimated with the ash residue method as γ_{ARM}). All other decomposition indicators we are aware of have only been used to estimate qualitative differences in the degree of decomposition of peat (Biester et al., 2014; Zaccone et al., 2018). Problems in the application of decomposition indicators are that the exact relation to γ is unknown, that confounding variables are known to weaken or to reverse the relation to γ, or worse, potential confounders are unknown, and that the values of decomposition indicators may be highly variable already for undecomposed peat because of differences in litter chemistry (e.g., Biester et al., 2014; Scheffer et al., 2001; Limpens and Berendse, 2003; Mahdiyasa et al., 2022; Broder et al., 2012; Stuart, 2004; Teickner and Knorr, 2022).

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To address these problems with measuring γ, we suggest to define properties of an ideal decomposition indicator and based on this develop a decomposition indicator that has these properties. An ideal decomposition indicator is linearly related to γ, well tested against litterbag data, does not confound differences in litter chemistry of undecomposed litter with decomposition, and is robust against other potential confounding factors, in particular mineral contents and mixing different litter types.

To develop such a decomposition indicator, we suggest to develop a model that predicts γ measured in litterbag experiments from mid-infrared spectra (MIRS). Predictions by these models are the suggested decomposition indicator, γ_{MIRS}. Such a model may fulfill the requirements of an ideal decomposition indicator because MIRS from litterbag experiments contain information about the relative abundance and interactions of many molecular structures (Stuart, 2004) which change in abundance during decomposition and differ between plant species (e.g., Arsenault et al., 2024a; Chapman et al., 2001; Cocozza et al., 2003; Tfaily et al., 2014). In contrast to other decomposition indicators that use simple formulas and no training data, such as C/N or humification indices, using a statistical model and undecomposed litter from various species as reference should avoid confounding differences in the chemistry of undecomposed litter with differences in chemistry due to decomposition. In contrast to γ_{ARM}, no knowledge of initial states is required because γ is predicted only with information from the decomposed sample. Previous studies used MIRS to predict various peat properties (e.g., Artz et al., 2008; Chapman et al., 2001), but, to our knowledge, not γ.

Peat samples can be much more complex than samples used in typical litterbag experiments because peat can be a mixture of multiple components: 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. Therefore, it will be important not only to evaluate γ_{MIRS} with homogeneous litter data, but also to evaluate γ_{MIRS} for mixtures of litter types similar to peat samples. To generate a diverse set of mixtures, one can add spectra of litterbag samples multiplied by scale factors. According to the Beer-Lambert law and with constant path length, these scale factors are the mass fractions of the components (Stuart, 2004) because MIRS intensities are proportional to the relative abundance of molecular structures and the relative abundance of a molecular structure is a weighted average of the relative abundances of the molecular structure of all components, where weights are the components' mass fractions. Also γ can be calculated for these mixtures from γ of the individual components and the initial litter masses, which allows us to test γ_{MIRS} for peat samples.

Theoretical considerations suggest that γ_{MIRS} will underestimate γ for mixtures of litter types: whereas both MIRS intensities and γ are weighted averages of the components' values, the weights are not the same. For MIRS intensities, the weights are the mass fractions of the components in the sample, as mentioned above, whereas for γ, the weights are the mass fractions of the components in the undecomposed sample. This difference also propagates to γ_{MIRS} predictions:

$$\begin{aligned} \gamma_{\text{MIRS}}(t) &= f^{-1}\left(\beta_0 + \sum_{k=1}^{K}\sum_{w=1}^{W}\beta_w h\left(I_{k,w}(t)\frac{m_k(t)}{m(t)}\right)\right) \\ \gamma(t) &= 1 - \frac{m(t)}{m(t_0)} = \sum_{k=1}^{K}\gamma_k(t)\frac{m_k(t_0)}{m(t_0)}, \end{aligned} \tag{1}$$

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where t_0 is the time when the sample was undecomposed, t is some time point later than t_0, k and w are indices for the component and wavenumber, $I_{k,w}(t)$ is the MIRS intensity at wavenumber w in component k, $m_k(t)$ and $m_k(t_0)$ are the mass and initial mass of component k, $m(t)$ and $m(t_0)$ are the mass and initial mass of the mixture, f^{-1} is the inverse link function of the prediction model for γ_{MIRS}, where we assume that the model is linear on the link scale with intercept β_0 and coefficients β_w for each wavenumber, and h is a transformation of raw intensity values due to spectral preprocessing (for example standard normal variate (SNV) normalization and z-transformation of predictors). Therefore, more decomposed components have a smaller weight for γ_{MIRS} than for γ, suggesting that $\gamma_{\text{MIRS}} < \gamma$, unless all components have the same γ or the sample consists only of one component.

If the bias is not negligible, alternative strategies to accurately estimate γ also for peat samples to the direct measurement of γ with γ_{MIRS} need to be developed. When γ_{MIRS} accurately estimates γ for individual litter types and h is a function such that $h\left(I_{k,w}(t)\frac{m_k(t)}{m(t)}\right) = h(I_{k,w}(t))\frac{m_k(t)}{m(t)}$, then it should be possible to estimate γ_{MIRS} for mixtures from $\gamma_k(t)$ for each component k as:

$$\gamma_{\text{MIRS}} = f^{-1}\left(\beta_0 + \sum_{k=1}^{K}(f(\gamma_k(t)) - \beta_0)\frac{m_k(t)}{m(t)}\right) \tag{2}$$

At first glance, it does not seem helpful to estimate $\gamma_{\text{MIRS}}(t)$ from $\gamma_k(t)$ to estimate $\gamma(t)$, but many peat samples consist of one or few dominant components which then also dominate the value of $\gamma(t)$. Using equation (2) in a mixing model (e.g., Cotrufo and Pressler, 2023) then allows us to estimate $\gamma(t)$ from $\gamma_{\text{MIRS}}(t)$ and we even get estimates for $\gamma_k(t)$ for free. Such a mixing model works when we know the mass fraction of each component ($m_k(t)/m(t)$). To analyze existing data, we suggest to approximate $m_k(t)/m(t)$ from the volume fractions in macrofossil analysis, as is also assumed in current peatland models (e.g., Frolking et al., 2010; Tuittila et al., 2013; Quillet et al., 2015). The same strategy also works when integrating γ_{MIRS} into peatland models. We note that theory also suggests similar biases for other decomposition indicators (that measure a property of the decomposing organic material), were these indicators used to estimate γ. Therefore, the bias is a general limitation when we attempt to estimate γ.

Here, we address the problems of estimating γ of individual litter types and peat, and the question whether it is possible to estimate γ of individual litter samples and of peat with γ_{MIRS}. In this context, our aims are:

1. To develop a novel decomposition indicator, γ_{MIRS}, which we define as γ, as measured in litterbag experiments, predicted from MIRS with a spectral prediction model.

2. To evaluate how well the developed models predict γ for peat samples as mixtures of litter types from (1) different species, (2) with different degree of decomposition, and (3) with admixtures of silicate minerals.

3. To develop a simple mixing model that allows to estimate γ of peat samples from bulk measurements and macrofossil volume fractions.

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4. To illustrate and discuss how γ_{MIRS} can be used to address open questions in peatland research (including the relation between saturated hydraulic conductivity and γ), to improve process models, to reconstruct past NPP, and to define site-specific references for γ and NPP for peatland restoration.

To this end, we collected available data from undecomposed litter and litterbag experiments for which MIRS and measurements of some commonly used decomposition indicators are available. This enabled us to compute beta regression models that predict γ from MIRS. Several models are computed because MIRS can be preprocessed in different ways and this may lead to differences in prediction errors and robustness. We evaluated the models on individual litter types using cross-validation and residual plots versus N contents, a known confounder of predictions from MIRS models (e.g., Teickner and Knorr, 2022). To evaluate applicability to peat samples, we apply the models to three sets of mixed spectra: mixtures of undecomposed material from different species, mixtures of material from different species and with different degree of decomposition, and mixtures of litter with a silicate-rich peat sample. Here, we test whether γ_{MIRS} underestimates γ for mixtures of litter types as predicted by the theoretical model in equations (1) and (2). Based on this analysis, we develop strategies to avoid this bias and show how γ_{MIRS} can be used to estimate γ and reconstruct past NPP for peat cores.

By developing and evaluating models that predict γ of litter from MIRS, we contribute to the development of a method that allows to accurately estimate γ of peat, therefore to better understand decomposition processes, reconstruct past NPP, and improve process models. This will contribute to a better understanding of peat accumulation processes, the definition of ecological baselines, and prediction of future peatland dynamics.

2 Methods

2.1 Training data

For our analyses, we used the following litterbag data: *Sphagnum capillifolium* (capitulum and first 5 cm of the stem) and *Typha latifolia* (leaves) samples incubated in bog peat and pools (oxic and anoxic conditions) in Canada (Arsenault et al., 2024a, b), and *Phragmites australis* (leaves and rhizomes) grown under different nutrient availability and incubated under anoxic conditions in peat with different nutrient availability (Reuter et al., 2019a, b, 2020). In addition, we used undecomposed litter samples (some collected under natural conditions, some grown in laboratory experiments with different nutrient availability) of *Astelia pumila*, *Aulacomnium palustre*, *Betula populifolia*, *Calluna vulgaris*, *Chamedaphne calyculata*, *Donatia fascicularis*, *Empetrum nigrum*, *Empetrum rubrum*, *Eriophorum angustifolium*, *Eriophorum sp.*, *Eriophorum vaginatum*, *Gaultheria antarctica*, *Isolepis setacea*, *Juncus effusus*, *Kalmia angustifolia*, *Larix laricina*, *Lepidothamnus fonkii*, *Polytrichum strictum*, *Rhododendron groenlandicum*, *Sphagnum capillifolium*, *Sphagnum fallax*, *Sphagnum magellanicum*, *Sphagnum rubellum*, *Sphagnum sp.*, *Tracheophyta*, *Vaccinium myrtilloides*, *Vaccinium myrtillus*, *Vaccinium oxycoccos*, *Vaccinium uliginosum*, and *Vaccinium vitis-idaea* (Wagner, 2013; Anzenhofer, 2014, unpublished; Hömberg, 2014; Agethen and Knorr, 2018; Mathijssen et al., 2019; Moore et al., 2019; Boothroyd et al., 2021; Worrall, 2021) from the pmird database (Teickner et al., 2025a). For undecomposed litter samples, we assumed a degree of decomposition of 0%. In total, 169 litter samples were available for

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model training. All MIRS used in this study are measured in transmission mode on Fourier-transform infrared spectrometers (FTIR) as milled samples mixed with potassium bromide into transparent pellets. MIRS were measured on different devices (Cary 660 FTIR spectrometer (Agilent, Santa Clara, CA, USA), Bruker Vector 22 FTIR spectrometer (Bruker Optik, Ettlingen, Germany), Cary 600 FTIR spectrometer (Agilent, Santa Clara, CA, USA), Varian 660 FTIR spectrometer (Agilent, Palo Alto, USA), Cary 670 FTIR spectrometer (Agilent, Santa Clara, CA, USA), and Shimadzu IRTracer-100 spectrophotometer, equipped with a DLaTGS (deuterated L-alaninedoped triglycine sulfate) detector).

2.2 Peat data

To evaluate the models and to illustrate the application of γ_{MIRS}, we used bog peat core measurements derived from the pmird database: a core from the peatland Odersprungmoor (OD2) (Gałka et al., 2022a), a core from the peatland Martinskapelle (MK1) (Gałka et al., 2022b), and a core from the peatland Mohoş (MH1) (Diaconu et al., 2020). Macrofossil volume fractions from these cores were used to estimate the mass fractions of individual litter components in the peat samples and average water table depth reconstructed from testate amoebae (TA-WTD) were used to relate estimated γ and NPP to changes in WTD. Age-depth models were estimated with ^{14}C dates using rbacon (Blaauw et al., 2017) (supporting section S1). In addition, we also used data from three ombrotrophic Patagonian peat cores from Broder et al. (2012) and two bog peat cores with highly degraded drainage layers from the Venner Moor to evaluate prediction domains of the models (see subsection 2.4.2).

2.3 Prediction model development

We used beta regression models to predict γ from intensities in preprocessed MIRS. To harmonize the spectra, we interpolated them to unit wavenumber resolution and clipped them to the range 600 to 4000 cm^{-1}. Depending on the variable and properties of the MIRS, different preprocessing steps may maximize predictive performance. Therefore, we computed models with different preprocessing steps in addition to the harmonization: (1) Baseline correction, signal normal variate (SNV) (model 1), (2) First derivative spectra, SNV (model 2), (3) Second derivative spectra, SNV (model 3). After that, spectra were binned (bin width 10 cm^{-1}) to reduce the number of predictors and reduce correlation between predictors, and all predictors were z-transformed across all spectra. All preprocessing steps were performed with the ir package (Teickner, 2022). Baseline correction was done with an automated convex hull procedure (Beleites and Sergo, 2021). Spectra of some undecomposed litter samples have artefacts from CO_2, as indicated by peaks around 2360 cm^{-1} (Wallace and NIST Mass Spectrometry Data Center, 1997). To avoid that these peaks have an effect on the normalization or models, we linearly interpolated intensities between 2300 and 2380 cm^{-1} and excluded variables from this range from the models. CO_2 also produces peaks around 670 cm^{-1} and 3580 to 3780 cm^{-1}, but we did not correct these because they overlap with peaks from organic matter and are smaller than the peaks between 2300 and 2380 cm^{-1} (Wallace and NIST Mass Spectrometry Data Center, 1997).

Beta regression models were computed with brms (Bürkner, 2018), using a logit link function, assuming a constant shape parameter, using a normal prior for the intercept, and regularized horseshoe priors (Piironen and Vehtari, 2017a, b) for the slopes (for each predictor variable). The regularized horseshoe prior shrinks coefficients to zero except where they are strongly related to the response variable, conditional on other predictors. To reduce overfitting, we defined a large amount of shrinkage, by as-

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suming that 5 of the 321 predictor variables have non-zero coefficients (Piironen and Vehtari, 2017b). Bayesian inference was done using Markov Chain Monte Carlo (MCMC) sampling with Stan (Stan Development Team, 2021), using 2000 warmup iterations and 2000 sampling iterations. Across all models, the maximum Monte Carlo standard error (Vehtari et al., 2021) for the degree of decomposition predicted for the training data and all analyzed peat samples was 1.1% for the mean, 0.5% (for standard deviations), and 4% (for lower and upper 95% prediction interval boundaries). No model had divergent transitions and the largest rank-normalized $\hat{R}$ for model parameters was 1.01, indicating convergence of the chains (Vehtari et al., 2021).

2.4 Model evaluation for litter samples

2.4.1 Prediction errors for individual litter types

We estimated the predictive accuracy of the models with 10-fold cross-validation (CV). CV folds were defined in two ways to evaluate predictive performance for two scenarios. In the first scenario, we used stratified CV, where each observation is assigned to a categorical variable and observations are split into the 10 folds while approximately preserving relative category frequencies. Each observation was assigned to a category based on the study and species, or, for samples from Reuter et al. (2019a), based on the study, species, and the site where the litter was grown (to balance occurrence of rhizome litter with different nutrient contents). This procedure approximates a test of the models with samples similar to the training data, as far as this is possible with our small and heterogeneous dataset.

In the second scenario, we used grouped CV, where each observation is assigned to a categorical variable and observations for the same categorical variable all are assigned to the same fold. The categorical variable was the same as for the stratified CV. This estimates predictive performance for novel litter types that are not part of the training data, for example the only litterbag data with *Sphagnum* litter is from Arsenault et al. (2024a), and therefore in this scenario a model not trained on decomposed *Sphagnum* litter predicts the degree of decomposition for decomposed *Sphagnum* litter. The procedure also implies that some folds only contain undecomposed litter because there are fewer categories for litterbag data than CV-folds. The purpose of this second scenario is to test model robustness for novel litter types.

To compare models, we used the expected log predictive density (ELPD) computed on observations held out during CV. Model evaluation was performed with the loo package (Vehtari et al., 2019). Following rules of thumb (Sivula et al., 2022), we assumed models to have equivalent predictive performance (according to the capability of our evaluation) when the difference of their ELPD (ΔELPD) is smaller than 4, and otherwise when ΔELPD is larger than two times its standard error (using normal approximation for ΔELPD). To give an easier to interpret performance metric, we also computed the root mean square error (RMSE).

2.4.2 Prediction domain coverage

We analyzed what fraction of the analyzed peat samples is within the prediction domain of the models. The prediction domain of a model (based on Wadoux et al. (2021), defined in Teickner and Knorr (2025)) is the range of the predictor variables covered by the training data. A sample is within the prediction domain if its preprocessed spectrum is within the range for each

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predictor variable, otherwise it is outside the prediction domain. If a sample is outside the prediction domain, it has spectral properties that cannot be interpolated from the training data and therefore the model extrapolates when making predictions for the spectra. In particular with models that overfit, this may lead to larger prediction errors than fitting errors for the training data.

2.4.3 Relations of model residuals to N content

We analyzed whether residuals are related to the nitrogen (N) content as proxy for proteins because it is known that protein content differs between species and increases during decomposition (Reuter et al., 2020; Scheffer et al., 2001; Limpens and Berendse, 2003; Biester et al., 2014), and that proteins, despite their comparatively small amount in peat, are a main control of the height and shape of peaks that are also caused by aromatics (Stuart, 2004). Thus, if one considers that the training data contains decomposed litter only from three species, the fit of the models may be confounded by proteins and this may bias predictions, especially under extrapolation. For some of the litter samples, no N measurements were available. For these samples, we predicted N contents from MIRS using prediction models from the irpeatmodels package (Teickner, 2025a; Teickner and Knorr, 2025). MIRS-predicted N contents are labelled N_{MIRS} and we indicate whether predictions are within the training prediction domain of the model (Teickner and Knorr, 2025).

2.5 Model evaluation for mixtures of peat components

2.5.1 Admixtures of minerals

The impacts of minerals on the estimated degree of decomposition was evaluated by adding a scaled version of a spectrum of a peat sample from the pmird database (Drollinger et al., 2019, 2020) with large mineral content (0.47 g g^{-1}, computed from loss on ignition; based on the mid-infrared spectrum (Fig. S6), many of them are silicates (Stuart, 2004; Parikh et al., 2014)) to selected spectra from the training data from different taxa and with different degree of decomposition. A range of scaling factors from absence of silicates to a clear dominance of silicates was chosen and we predicted the degree of decomposition for each spectrum created this way. For the same samples from the training data, we evaluated the impact of adding increasing amounts of a very decomposed sample (based on $HI_{1630/1090}$, peat structure, C content, and degree of decomposition predicted by all models).

2.5.2 Mixtures of undecomposed and decomposed litter

To evaluate how robust the models are for mixtures of litter from different taxa and with different degree of decomposition, we created pairwise mixtures from two sets of spectra. The first set consisted of randomly selected undecomposed litter samples from 15 taxa and the two most decomposed samples per taxon (where available). The spectra in this set were scaled in the range 0.001 to 1000. The second set consisted of the two most decomposed samples and the least decomposed sample per taxon, which are not already in the first set. All pairwise mixtures of the spectra from the first and second set were created and γ_{MIRS} predicted with all three models. Values of γ were computed with equation (1). The value of $\gamma_k(t)$ is measured in the

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litterbag experiments, the value of $m_k(t_0)$ is computed by assuming that the scale factors correspond to masses (as outlined in the Introduction) as: $m_k(t_0) = m_k(t)/(1-\gamma_k(t))$. Values of $m(t)$ are computed as sum of the scale factors of the components. We then used $\gamma(t)$ measured for each component and equation (2) to estimate γ_{MIRS} to test whether this theoretical model can reproduce γ_{MIRS} for the mixtures, irrespective of the litter type.

To evaluate in more detail how robust the models are for mixtures of undecomposed litter, we selected one sample per taxon from the undecomposed litter samples and created all pairwise mixtures with equal amounts of of both components. It was tested whether predictions of the models for these mixtures match the expected value for γ of 0 g g^{-1}.

2.6 Estimation of γ for peat cores from bulk measurements of $\gamma_{\text{MIRS}}(t)$ and reconstruction of past NPP

We developed a simple Bayesian mixing model based on equation (2) that estimates $\gamma_k(t)$ for all components in a peat sample from bulk measurements of $\gamma_{\text{MIRS}}(t)$ (predicted by any of the three models) and the mass fractions of the components:

$$
\begin{aligned}
\gamma_{\text{MIRS}} &\sim \text{beta}(\mu_{\gamma_{\text{MIRS}}}\phi_{\gamma_{\text{MIRS}}}, (1-\mu_{\gamma_{\text{MIRS}}})\phi_{\gamma_{\text{MIRS}}}) \\
\mu_{\gamma_{\text{MIRS}}} &\sim \text{beta}(\mu\phi, (1-\mu)\phi) \\
\mu &= \text{logit}^{-1}\left(\beta_0 + \sum_k^K (\text{logit}(\gamma_k) - \beta_0)\frac{m_k}{m}\right) \\
\phi &\sim \text{gamma}(\alpha_\phi, \beta_\phi) \\
\gamma_k &\sim \text{beta}(\alpha_{\gamma_k}, \beta_{\gamma_k}) \\
\beta_0 &\sim \text{normal}(\beta_{0_\mu}, \beta_{0_\sigma})
\end{aligned}
\tag{3}
$$

where the third line is the same as equation (2), the first line is a measurement error model to consider prediction errors in γ_{MIRS} (here, we approximate errors of the prediction model with a beta distribution with scale parameter $\phi_{\gamma_{\text{MIRS}}}$ computed from the average prediction error of the respective model), μ is the estimated true value of γ_{MIRS} (without measurement errors), ϕ is the scale parameter of the beta distribution (with a gamma prior with shape and rate parameters α_ϕ, β_ϕ), and γ_k of component k is modeled with a beta distribution with shape and rate parameters α_{γ_k} and β_{γ_k}. As outlined in the Introduction, linking this model to peat core data can be done with bulk measurements for γ_{MIRS} and by assuming that m_k/m equals the macrofossil volume fractions of the litter components. For individual litter types, the mixing model will only yield correct estimates for γ_k when they have a relatively large mass fraction because γ_{MIRS} is not sensitive to γ_k if component k has only a small mass fraction. To consider this error source, we used a beta$(1,1)$ prior for γ_k, which gives uniform weights to all possible values. Unless the sample consists of many components, the inability to correctly estimate γ_k for components with small mass fraction in the sample has only a small effect on γ and an even smaller effect on the reconstructed NPP. We expect large errors not accounted for by the mixing model only when some initially dominant component is completely or nearly completely decomposed and therefore not detectable.

We applied this model to the three cores, OD2, MK1, and MH1 described in section 2.2 to estimate γ_k of all K litter components

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and the γ of the peat samples. With these estimates for γ_k, bulk densities estimated from MIRS (Teickner and Knorr, 2025; Teickner, 2025a), and age-depth models for each core, we could then estimate the initial mass of each layer, which divided by the time range of aboveground litter formation in each layer without roots equals the aboveground NPP. Reconstruction of belowground NPP is only possible with peatland models. Our analysis considers errors in estimates for γ_{MIRS}, bulk density, peat ages, and β_0. We also developed an R package that allows to estimate the mixing model for own data (Teickner, 2025b).

2.7 Relation between saturated hydraulic conductivity and γ

Using the estimated γ for the peat samples and saturated hydraulic conductivity (K_{sat}) estimated from MIRS (Teickner, 2025a; Teickner and Knorr, 2025), we tested whether K_{sat}-γ relations hypothesized in previous studies agree with K_{sat} and γ for our peat cores. The hypothesized relations are:

1. An assumed sigmoidal relation as used in the Holocene Peatland Model (corrected versions of equations (10) and (15) in Frolking et al. (2010); corrected versions are available from the supporting info to Treat et al. (2022), K_{sat} in cm min^{-1}, according to Morris et al. (2015a)):

$$K_{\text{sat}} = \frac{150}{70} - \frac{3}{70}\left(\rho_{\text{min}} + \Delta\rho\left(1 - 0.5\left(1 - \text{erf}\left(\frac{(1-\gamma) - c_3}{\sqrt{2}c_4}\right)\right)\right)\right), \tag{4}$$

   where ρ_{min}, $\Delta\rho$, c_3, and c_4 are parameters defined in Frolking et al. (2010) and erf is the error function.

2. An assumed exponential relation (Morris et al., 2011) as used in the DigiBog model (Morris et al., 2012):

$$K_{\text{sat}} = 0.001\exp(8(1-\gamma)) \tag{5}$$

3. An empirical relation that was developed with γ estimates derived from C/N ratios (Morris et al., 2015a):

$$K_{\text{sat}} \approx 1.2(1-\gamma) + 2.6147\ \text{depth} - 0.877\ \text{hollow} - 0.020\ \text{center} - 2.87, \tag{6}$$

   where depth is the mid depth of a layer, hollow is a dummy variable which is 1 when the layer is from a hollow, and center is a dummy variable which is 1 when the layer is from the center of the peatland (in our calculations, we use depth $\in \{0.3, 0.5\}$ m, hollow $= 0$, and center $= 1$).

3 Results

3.1 Predictive performance

All models have a similar fit to the training data (Fig. 1) and similar predictive performance as measured by their ELPD during CV (Tab. 1). Model 2 had the best average predictive accuracy (= maximum average ELPD) for the stratified CV and model

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1 for the grouped CV. Using a normal approximation for ΔELPD and a two-sided significance level of 5%, only model 3 in the stratified CV has a detectably worse predictive accuracy than the model with best average ELPD (Tab. 1). Large errors of ΔELPD in the grouped CV indicate a large variability in predictive performance of the model for the different folds, as expected when testing the model with litter samples from species not included in the training data.

For all models, the fit to the training data is better on average (smaller average RMSE) than for predictions in the two CV scenarios (Fig. 1), indicating that all models overfit. The two models using derivative spectra had, on average, the best fit to the training data, but worse or not much better predictive accuracy in the CV scenarios, indicating an, on average, larger overfitting risk than for model 1, which does not use derivative spectra.

Predictive accuracy of all models was worse for the grouped CV than for the stratified CV (Fig. 1), as expected, because in the stratified CV models were tested with samples from similar studies and species as the data they were trained with, whereas in the grouped CV some folds contained samples from species the model was not trained with. In the grouped CV, γ is underestimated by all models for decomposed *T. latifolia* and *S. capillifolium* samples from Arsenault et al. (2024a). Conversely, γ is overestimated for undecomposed litter samples, with prediction errors larger than 10% for model 1 for *C. vulgaris*, and for the other two models for *L. fonkii*, *C. vulgaris*, *P. australis*, *A. pumila*, *L. laricina*, and *C. calyculata*. Model 3 has, both in the grouped and stratified CV, the largest average prediction errors for undecomposed litter (Fig. 1).

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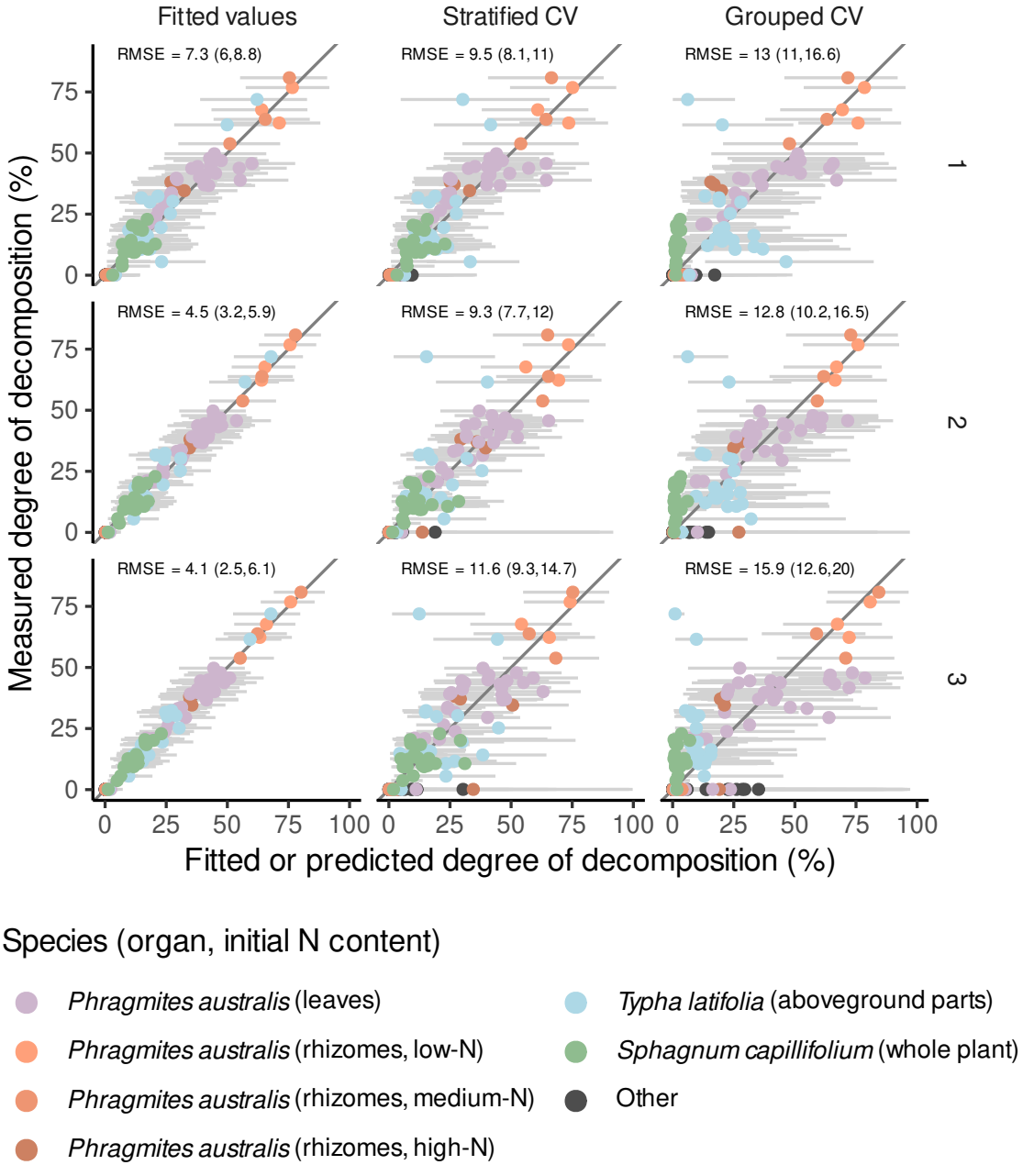

Figure 1. Fitted values (first column) or predictions for folds held out during CV for the two CV scenarios (second and third columns) versus the measured γ for the training data, for each model (rows). For litterbag data, different colors represent different taxa, for undecomposed litter all samples are labelled as "Other" and have the same color. For *P. australis* rhizomes from Reuter et al. (2020), we additional differentiate between initial N contents (low, medium, and high N content). Error bars are 95% prediction intervals. For each case, we give the average RMSE and lower and upper 95% confidence intervals computed from MCMC draws.

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Table 1. Difference of expected log predictive density of all models to the best model (ΔELPD) and corresponding standard error (SE(ΔELPD)) for stratified or grouped cross-validation. In each case, the best model is at the top.

Stratified CV			Grouped CV		
Model	ΔELPD	SE(ΔELPD)	Model	ΔELPD	SE(ΔELPD)
2	0.00	0.00	1	0.00	0.00
1	-17.56	9.24	2	-33.60	18.38
3	-34.49	9.55	3	-91.48	52.05

3.2 Prediction domain coverage

A comparison of the prediction domains of the models to the spectral range covered by the analyzed peat samples indicates that many of the peat samples have MIRS different to the training data. $HI_{1630/1090}$ as alternative decomposition indicator, C or C_{MIRS}, and photographs of the peat samples, suggest that samples outside prediction domains are either more decomposed or have large mineral contents (Fig. S4 and S5), which is not surprising since there are comparatively few decomposed samples and no mineral-rich samples in the training data. Data coverage by prediction domains differs between the models: 64.4% of the peat samples are within the prediction domain for model 1 and 2.8% and 0% for the other two models, which indicates that derivative spectra differ more between the peat and the training data data than underived spectra. Thus, the models extrapolate for more decomposed and mineral-rich peat and the prediction domain of model 1 covers most of the peat samples.

3.3 Relations of model residuals to N contents

A plot of residuals versus N for different levels of the γ suggests that model 1 underestimates γ for samples in the training data with a γ between ca. 20 and 40% and N content smaller than ca. 0.02 g g^{-1} (Fig. 2). For the models computed with derivative spectra, this bias is smaller (Fig. 2). This may indicate that model 1 makes less accurate predictions for the peat samples analyzed here (99% have a N content smaller than 0.02 g g^{-1}) and in general (Loisel et al., 2014).

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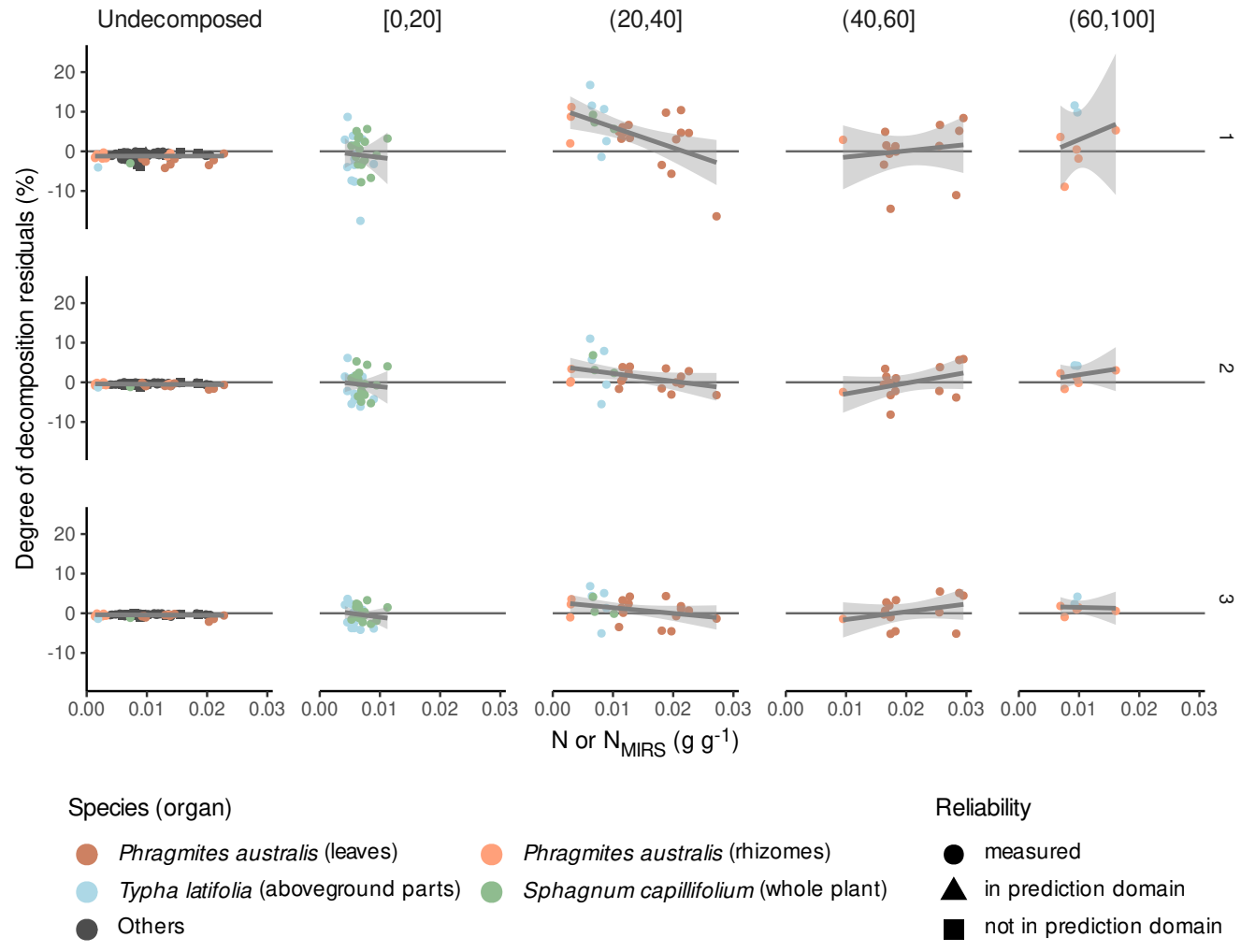

Figure 2. Model residuals (measured γ - γ_{MIRS}) versus N or N_{MIRS} for different levels of γ (columns) and the three models (rows). Points are averages and lines and shaded areas averages and 95% confidence intervals of regression models fitted to the average residuals. "Reliability" refers to how reliable the N or N_{MIRS} values are. Values of N_{MIRS} are less reliable when they are not in the prediction domain, which is the case only for some of the undecomposed litter samples.

3.4 Predictions with additions of a silicate-rich sample

For silicates, prediction errors of all models increase the more silicates are mixed into the samples such that 95% prediction intervals cover nearly the whole range of possible values for γ_{MIRS} (Fig. S7 to S9). The behavior of predicted medians differs between the models. For model 1, predictions overall increase for undecomposed samples and decrease for more decomposed samples, but the differences are never larger than ca. 30%. Model 3 behaves similar, but predictions always increase with

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more silicate influence and differences to the true value may exceed 50%. For model 2, predictions decrease with more silicate influence for all but the undecomposed samples and compared to the other models more posterior probability is placed on smaller degrees of decomposition.

3.5 Predictions with additions of strongly decomposed samples

For decomposed peat, the median predicted γ_{MIRS} increases for all samples and models, as expected when adding a highly decomposed peat sample to less decomposed litter samples (Fig. S10 to S12). Median predictions for the maximum addition of the decomposed peat are smallest for model 1 and largest for model 3. As for the silicate experiment, also prediction errors of all models increase the more of the decomposed sample is mixed into the samples, but prediction intervals are narrower than for the silicate experiment and, especially for already decomposed litters, their width also differs between models: Model 1 estimates the largest prediction errors and prediction errors increase the more of the decomposed peat is added to a sample, even for decomposed litter. Model 2 and in particular model 3 have narrower prediction intervals for already decomposed litter, but in most of the cases predictions do not differ significantly from those of model 1. Thus, model 1 estimates a smaller median γ_{MIRS} with larger prediction errors than the models using derivative spectra, but all models make extrapolations that are qualitatively reasonable.

3.6 Predictions for mixtures of different litter components

Predictions of all models for samples consisting of two litter types with different degree of decomposition underestimate γ. As shown in Fig. 3, the bias is well described by our theoretical expectation (equation (2)). Thus, the magnitude of the bias is related to the difference in γ of the mixed litter types and their relative mass fractions in the mixture. This relation is non-linear; when one of the two litter types is clearly dominant (mass ratio of 1:1000), the bias vanishes, such that for mass ratios in-between these extremes, the bias reaches a maximum. This maximum value is larger the larger the difference in γ between the two litter types is. The difference in γ also controls the position of the maximum. The more decomposed one of the components is compared to the other component, the more is the maximum shifted towards a smaller mass fraction of the more decomposed component.

There is some deviation from this pattern due to prediction errors in γ_{MIRS} for individual litter samples. Discrepancies not related to model prediction errors for individual litter types only occur when undecomposed litter of one species is mixed with strongly decomposed litter of some different species, where the mass ratio of the more decomposed litter type is between one third and two thirds (upper right and lower left panels in Fig. 3, where diverse litter types are mixed with *P. australis* and where *S. capillifolium* litter is mixed with *P. australis* litter). If only undecomposed litter from different species and organs is mixed, γ_{MIRS} correctly estimates a small γ (values range between 0 and 0.02 g g^{-1} across all mixtures and models), which is also in line with our expectation. Overall the bias is similar across all models and for mixtures of different species and organs, and can be well described by equation (2), with smaller deviations caused by prediction errors for γ_{MIRS} and variation between litter types. The bias estimated with model 2 matches the expected relation best.

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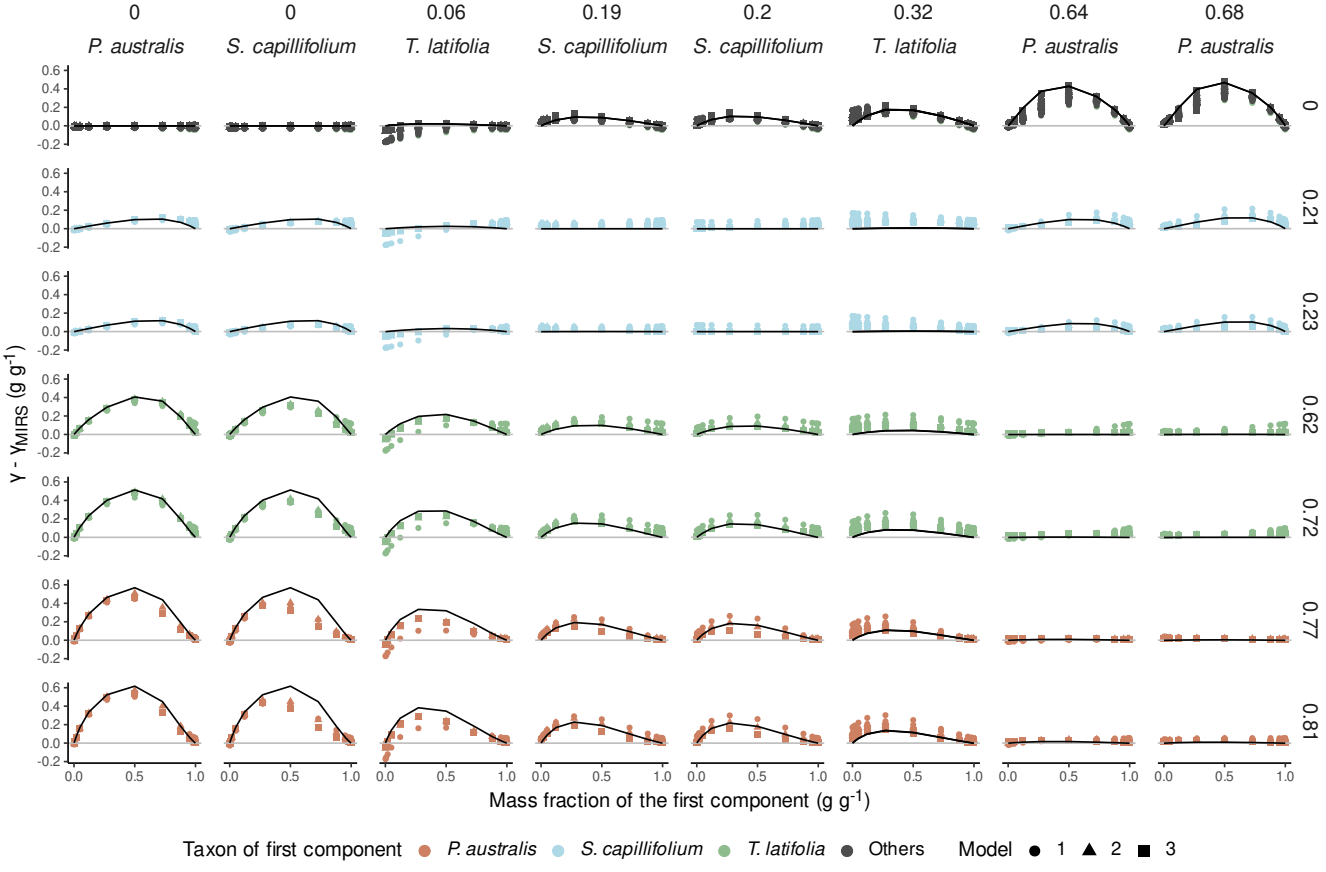

Figure 3. Values of γ minus γ_{MIRS} (predicted by all three models) for mixtures of two litter types (components) versus the mass fraction of the first component. Columns indicate the second component of the mixture (indicated by γ and species) and rows indicate the first component of the mixture (indicated by γ). Point colors indicate the species of the first component. Point shapes indicate the model with which γ_{MIRS} was predicted. The black lines are calculated with equation (2) using average coefficients from model 1.

3.7 Degree of decomposition and reconstructed NPP for peat cores

Figure 4 shows γ and NPP of individual litter types estimated with γ_{MIRS} and the average γ and total aboveground NPP for the three peat cores versus time. For MH1, γ was smaller than 50% throughout the last 500 years; larger values values were only estimated for two short phases around 1700 and in the last decades, where *S. cuspidatum* and *E. vaginatum* dominated and TA-WTD indicate drier conditions. The reconstructed median NPP at MH1 is larger than at the two other sites, the median was stable during the last 500 years and larger than 0.1 kg m^{-2} yr^{-1}. Recent and past drying events coincide with a decrease in NPP. For MK1, the oldest core, the median γ is ca. 75% for the fen phase and peat formed during 500 to 1800 CE, but similarly small as for MH1 for the intermediate layers dominated by hummock *Sphagnum* species (model 3 predicts a larger γ here than the other two models). The NPP was similarly large as in MH1 only in the fen phase and much smaller (median

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smaller than 0.15 kg m^{-2} yr^{-1}) afterwards. No fen phase is covered by OD2 and γ was small and more stable than in the other cores, with only a small peak roughly during the period of the Little Ice Age. The NPP was similar to MK1. In contrast to all other cores the NPP strongly increased during the last decades in OD2. In many cases, the apparent mass accumulation rate (AMAR) is nearly identical to the reconstructed NPP, but AMAR underestimates the median NPP and decomposition mass losses for more decomposed layers. Many decomposition peaks appear to be related to peaks in reconstructed WTD (drying events) (for example MH1: ca. 1700 CE and in recent decades, MK1: ca. 1700, 1500, 1000 BCE, OD2: ca. 2700, 1700, 700, 400 BCE), but there are also WTD peaks that do not coincide with an increase in γ (also not when possible time lags between WTD and γ are considered, for example: MK1: ca. 3000 BCE, OD2: ca. 700 CE).

Common patterns between all models and cores are that dominance of *Eriohporum* sp. in peat often coincides with a large γ, that a small γ is estimated for the topmost layers (as expected), and that a rather small γ ($< 50\%$) is estimated for many *S. fuscum*, *S.rubellum*, and *S. magellanicum* layers even though they are several thousands of years old (and similarly, the overall γ for these layers). The dominance in *Eriohporum* is often preceded by an increase in γ of *Sphagnum* peat (e.g., MK1: ca. 1300 BCE, OD2: ca. 700 and 0 BCE) and γ often only decreases after *Eriohporum* volume fractions are smaller again. This pattern is compatible with secondary decomposition and colonization by *Eriohporum* caused by drier conditions.

While the models indicate overall similar trends in γ and NPP, values of γ and NPP vary comparatively much between the three models: model 1 estimates the smallest γ and NPP, model 3 the largest values, and model 2 estimates intermediate values. Model 3 does, for example, not estimate a decrease in γ for MK1 during ca. 5000 to 4500 BCE. However, the estimated maximum values of γ per core are similar. Overall, model 3 suggests a smaller average difference in γ between phases with more decomposition losses and phases with less decomposition losses than the other two models. Large errors in γ are mainly due to extrapolation for more decomposed samples. Large errors in NPP are mainly due to dating errors (unlike many studies, we considered these errors here).

Our estimates for *S. fuscum* NPP cover the range of NPP from different studies compiled by Bona et al. (2018) (0.12 ± 0.09 kg^{-1} yr^{-1}, average $\pm$ standard deviation) (Moore, 1989; Reader and Stewart, 1972; Rochefort et al., 1990; Szumigalski, 1995; Thormann and Bayley, 1997), and are contained in the wider NPP range measured in monospecific *S. fuscum* patches in Bengtsson et al. (2021) (0.21 ± 0.14 kg^{-1} yr^{-1}) (Bengtsson et al., 2020) or other studies (Wieder et al., 2016, 2019). While it is not surprising that our estimates are within these broad ranges, it is reassuring to see that median estimates produced with the suggested approach do not obviously contradict expected ranges for NPP.

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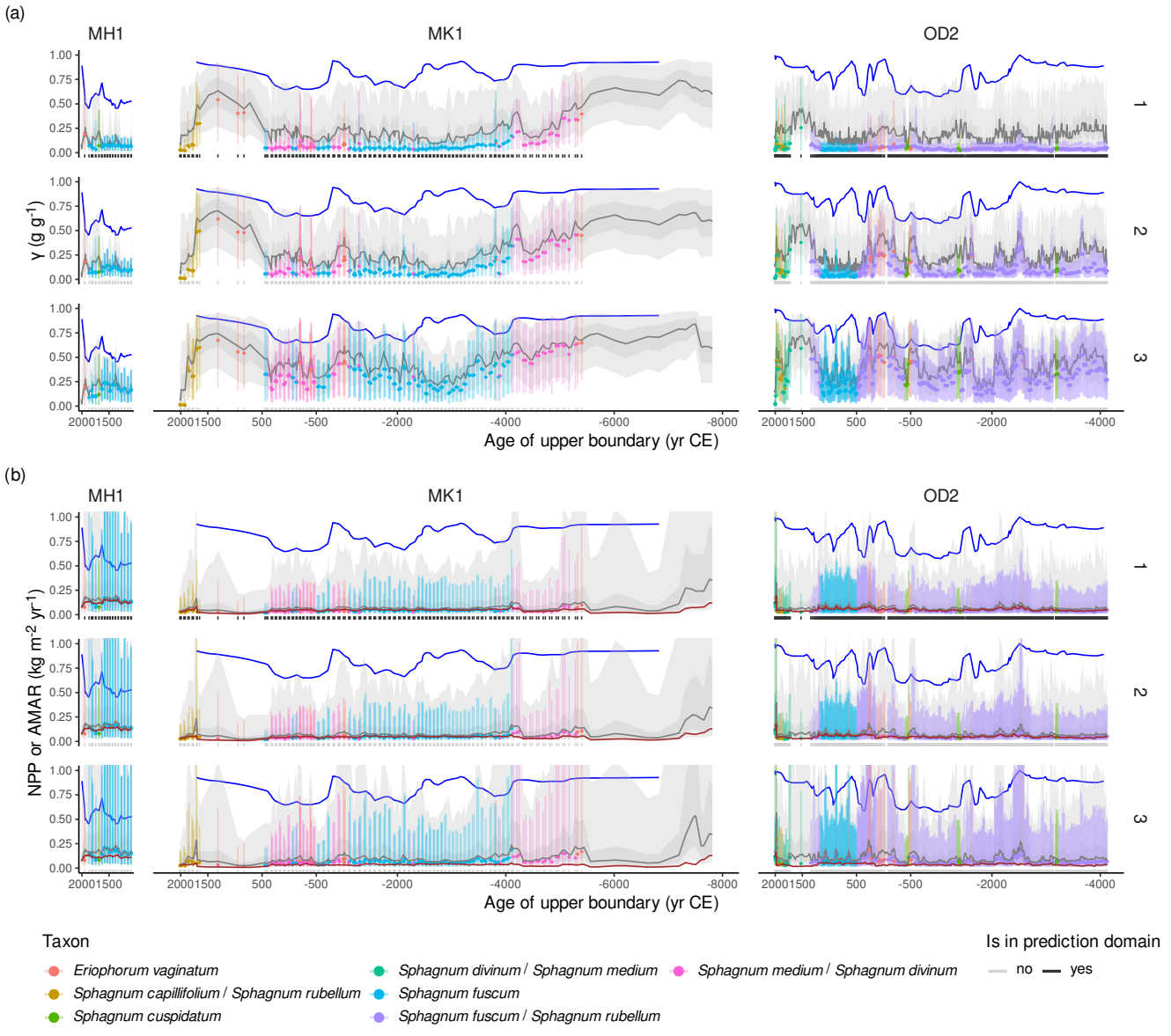

Figure 4. Reconstructions of γ and the NPP from γ_{MIRS} for the three peat cores analyzed here. Columns show results for peat cores and rows for the three prediction models for γ_{MIRS}. The x axis is the age of the upper boundary of the layers, measured since the coring date. Panel (a) shows γ estimated for taxa with a volume fraction of at least 40% in at least 15 samples (colored points are medians and error bars 90% confidence intervals) and the median γ of each layer (grey shaded areas and grey line; the grey shaded areas are 50% and 90% confidence intervals). Panel (b) shows the NPP (or, in presence of roots, the initial mass rate) for taxa with a volume fraction of at least 40% in at least 15 samples (colored points are medians and error bars 90% confidence intervals), the median NPP of each layer (grey shaded areas and grey line), and the median apparent mass accumulation rate (AMAR) (brown line). The y axis is clipped at 1 kg m^{-2} yr^{-1}. Blue lines are average reconstructed WTD (normalized). The color of the small rugs along the x-axis ("Is in prediction domain?") indicate whether the MIRS for the peat samples are within the prediction domain of the models for γ_{MIRS}.

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3.8 Relation between saturated hydraulic conductivity and γ

The estimated relation between MIRS-estimated saturated hydraulic conductivity (K_{sat}) and γ for the three peat cores and with γ estimated from γ_{MIRS} predicted by the three models is shown in Fig. 5, together with K_{sat}-γ relations suggested in earlier studies. At least for the cores analyzed here, default parameterizations differ from estimated averages (albeit one has to consider that both K_{sat} and γ estimates have relative large errors): In contrast to the relation implemented in the Holocene Peatland Model (equation (4)), the data suggest that K_{sat} decreases continuously with γ and our data do not cover ranges of γ large enough to test the suggested step-like decrease for strongly decomposed peat. The relation suggested in Morris et al. (2011) and used in the DigiBog model overestimates K_{sat} and estimates a too strong decrease of K_{sat} with γ. The relation suggested in Morris et al. (2015a) fits our estimates well, but the estimated depth dependence is too strong (for example, if a depth of 50 cm is assumed for all samples, K_{sat} would be underestimated, as shown in Fig. 5; in contrast our estimates suggest a less strong control of depth ($\approx$ total stress) on K_{sat} for our cores).

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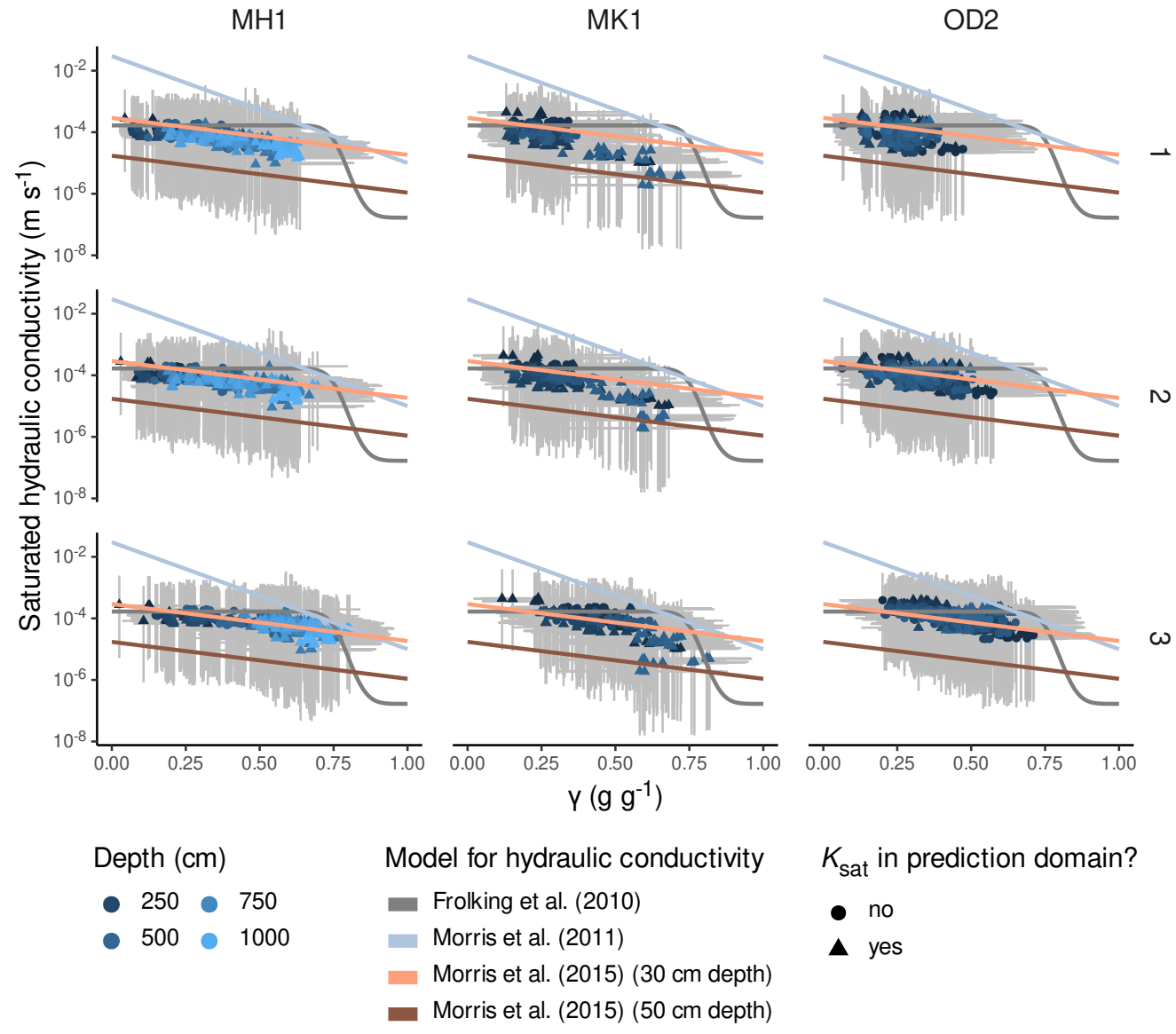

Figure 5. Relation between MIRS-predicted saturated hydraulic conductivity (K_{sat}) and γ for the three peat cores analyzed here (columns) and with γ_{MIRS} predicted by one of the three models (rows). Points are average estimates and error bars are 90% prediction intervals. Point colors indicate the depth of the peat layers. Point shapes indicate whether MIRS from which K_{sat} were predicted are within the training prediction domain of the model ("yes") or not ("no"). Predictions outside the prediction domain may have larger errors than estimated. The lines are K_{sat}-γ relations suggested in the literature (see the text for details).

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4 Discussion

To address the problem of estimating γ for peat samples, we developed and evaluated a novel decomposition indicator, γ_{MIRS}, and developed the mathematical tools necessary to estimate γ with γ_{MIRS} even for complex mixtures of several litter types with different γ. This enabled us to analyze in detail γ and the past NPP for three peat cores based on bulk MIRS. Overall, this suggests that the approach developed here is a promising first step towards accurate estimation of peat γ and reconstruction of past NPP. As is the case for all novel and complex prediction models, intensive testing is required to address remaining limitations and reduce prediction errors and some of this work remains to be done by future studies. The diverse palette of tests used here both shows that γ can be estimated with γ_{MIRS} with reasonably small errors for the various litter types considered here, and helps to identify limitations and possible future improvements.

In the next subsections, we synthesize the mixing model approach to compensate the bias in γ_{MIRS} for mixtures of litter types (subsection 4.1), we synthesize the evaluation of the prediction models, and we identify limitations which can be addressed in future studies (subsection 4.2). We also discuss how the approach developed here can be even further improved to estimate γ and reconstruct the NPP, how γ_{MIRS} can be linked to process models and what other research questions may be addressed and illustrate this with our analysis of the three peat cores (subsection 4.3).

4.1 Estimating γ from γ_{MIRS} for mixtures of litter types

As outlined in the Introduction, γ_{MIRS} is biased when litter types with different degree of decomposition are mixed. Our results suggests that equation (2) reasonably well fits γ_{MIRS} for mixtures of litter types; larger deviations only occur for litter mixtures that are probably rare under natural conditions (mixtures of one to two thirds of an undecomposed litter with a two to one thirds of a strongly decomposed litter). Moreover, at least for models 2, these deviations are small compared to prediction errors. Thus, since equation (2) reasonably well fits γ_{MIRS} for mixtures of litter types and since γ_{MIRS} fits γ of individual litter types well, the bias can be avoided or corrected.

There are three possible approaches to avoid or correct this bias: The first approach is to use bulk γ_{MIRS} measurements and information on the relative mass fractions of each litter type in the sample (for example from macrofossil analysis) to estimate γ from γ_{MIRS} with the mixing model (equation (3)) developed here; this corrects the bias. The second approach is to measure MIRS for the separate litter types and weigh the litter types (component-specific analysis). In these cases, γ_{MIRS} can be estimated for each litter type and, with reasonable prediction errors, equals γ. This can be used to estimate the initial mass of the litter types, $m_i(t_0)$, from γ_{MIRS} with: $m_i(t_0) = m(t_0)/(1-\gamma_{\text{MIRS}})$. Then, equation (2) can be used to compute γ of the entire sample; this approach avoids the bias. The third option is a combination of the first and section approach, where a component-specific analysis is conducted only for some litter types.

The second approach can be used to estimate γ more accurately, both for the sample and individual litter types, than is possible with the first approach This is particularly relevant for litter types that have only a small mass fraction because the mixing model cannot estimate γ very accurately for these litter types (for this reason we only analyzed litter types with a macrofossil abundance of at least 40% in the peat samples). Even though the sample γ is less sensitive to the values of litter types with

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small mass fraction than γ of these litter types, also estimates for the sample γ will have smaller errors. The third option shares this advantage and may be an option when it is difficult to separate all litter types (for example when litter types are strongly decomposed).

This points to a possible practical difficulty: it is not yet clear how to exactly define litter types and mass fractions such as to avoid biases. The mixing model and the component-specific analysis require litter types to be separated, but future studies will need to test which plant organs need to be separated to avoid biases. For example, it is quite clear that tree branches will decompose at a different rate than leaves and therefore both need to be treated as separate litter types to avoid biases. But does the same apply, for example, also to *Sphagnum* branches versus stems? Here, we assumed that macrofossil volume fractions are directly proportional to mass fractions, as is done in process models, but this assumption is not well tested. Peat layers may also consist of peat formed over a long time range that is strongly compressed and may therefore consist of not much decomposed parts and strongly decomposed parts. In such cases, it may not be sufficient to define litter types only via taxonomic information because litter from the same species may have a large range of γ values in such layers. On the other hand, component-specific analysis can be used to determine whether γ of two litter types is sufficiently similar throughout the decomposition process such that the bias in γ_{MIRS} is only small and both may therefore be treated as same litter type.

Overall, it is exciting to see that the possibility to estimate γ raises these issues and offers opportunities to test them and therefore to better understand peat chemistry and degree of decomposition.

4.2 Which properties of an ideal decomposition indicator does γ_{MIRS} fulfill and where are there still limitations?

The main question we want to address here is to what extent the prediction models for γ_{MIRS} fulfill the properties of an ideal decomposition indicator suggested in the Introduction and compared to previous studies:

1. **Linear relation to γ:** Our model evaluation suggests that all three models fit γ of individual litter types with reasonable errors and no overall bias (Fig. 1). For litter similar to the training data, prediction errors are comparable to or slightly larger than errors between litterbag replicates (e.g., Teickner et al., 2025c) and therefore currently acceptable for many applications. Predictions for novel litter types should be treated with caution since there might be biases (Fig. 1), however the dataset here already covers quite many different litter types and therefore we expect that this risk is small, except for woody plant organs which are currently underrepresented in the training data. Overall, γ_{MIRS} is linearly related to γ of individual litter types.

2. **Tested against litterbag data:** While there are gaps in our training data, we are not aware of other studies that test prediction of γ with decomposition indicators with an as diverse set of litter samples as done here.

3. **No confounding by differences in litter chemistry:** The models successfully fit γ for many diverse litter types. Whilst decomposed litter samples are underrepresented in the training data, undecomposed samples from many different taxa and all relevant plant functional types (non-*Sphagnum* mosses, *Sphagnum* mosses, sedges, herbs, shrubs, and trees) have a good fit in the model and, in most cases, also in the stratified CV. Also mixtures of different litter types are well

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predicted when the bias in γ_{MIRS} is compensated. Overall, this indicates that our models only have a small bias for different litter types.

4. **No confounding by minerals:** MIRS are strongly impacted by silicates. It will therefore be unlikely, at least with the simple linear prediction models developed here, to accurately predict γ from MIRS. For this reason, it is encouraging that γ_{MIRS} has large prediction errors when mineral contents increase; conversely to γ_{MIRS}, humification indices indicate a smaller γ for samples with mineral admixtures and therefore is biased by silicates.

5. **No confounding when mixing litter types:** While γ_{MIRS} is a biased estimator for γ for litter mixtures, this bias can be corrected, as discussed in the previous subsection. We also emphasize that such a bias is not specific to γ_{MIRS}, but is a property of any decomposition indicator that measures a property where weights when computing averages for samples depend on γ, which is the case for nearly all decomposition indicators (all we are aware of except for γ_{ARM}).

Predicting γ is a complex task and as any complex method, γ_{MIRS} has limitations, many of which can be addressed in future studies:

1. **Variability between models:** Currently, it is difficult to recommend a best model because the models have trade-offs that need to be evaluated with additional data. Our recommendation is to consider the variability of model predictions while taking into account known biases (see the next point) until further tests have been performed. While confidence intervals of γ estimated by the models overlap even for samples outside of the prediction domain, the large variability indicates that at least some of these predictions are biased. Overall, we assume that predictions of model 2 are most accurate because model 1 underestimates γ for litter with small N content and model 3 probably overestimates γ for more decomposed samples.

2. **Limitations of individual models:** Model 1 fits the data worst and underestimates γ most for *T. latifolia* and *S. capillifolium* samples with N content < 0.02 g g^{-1} and therefore probably underestimates γ for many peat samples and compared to the other two models. However, it has the best average predictive performance in the stratified CV, which we think best approximates possible applications of the models to peat samples, and it is also the model that confounds the least differences in initial litter chemistry with decomposition in the CV (Fig. 1).
   Model 3 overfits the data most, based on the stratified CV, and confounds the most differences in initial litter chemistry with decomposition in the CV (Fig. 1), but when trained on all data, it fits γ best and does not confound difference in the chemistry of decomposed litter with decomposition, and it does not underestimate the degree of decomposition for *T. latifolia* and *S. capillifolium* samples with N content < 0.02 g g^{-1}. For more decomposed samples, model 3 may overestimate γ, as indicated by high γ estimates in the analysis of the peat cores (Fig. 4) and underestimation of the theoretically expected bias for mixtures of undecomposed and very decomposed components (Fig. 3).
   In all aspects mentioned in the previous two points, model 2 is intermediate between the other two models and in addition has the best average predictive performance in the stratified CV (Fig. 1) and best compensates the bias for mixtures of litters (Fig. 3). However, even though 95% prediction intervals also cover the complete possible range for samples with

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large mineral contents, the median predicted degree of decomposition and bulk of the posterior distribution decrease the more silicates are within a sample, which means that γ is underestimated for samples with large silicate contents.

3. **Prediction domain coverage:** It would be useful to include material from more litter types (in particular woody plant organs) and samples with larger γ than is currently the case in order to reduce extrapolation errors of the models for decomposed peat samples.

4. **Confounding by carbonates:** We could not test whether γ_{MIRS} is biased by admixtures of carbonates which can be relevant in fen peat. It is likely that carbonate-rich samples confound γ_{MIRS} because peaks caused by carbonates interfere with peaks caused by aromatics and proteins (Tatzber et al., 2007).

5. **Modeling approach:** We used a modeling approach that is robust against overfitting with relatively small sample sizes, but there are more flexible modeling approaches (e.g., Viscarra Rossel et al., 2024) that may have smaller prediction errors or may better fit more diverse litter types or even make more accurate predictions for samples with minerals or carbonates. These modeling approaches need larger and more homogeneous datasets to avoid overfitting.

6. **Limitations of the mixing model:** We developed a simple mixing model that corrects the bias in γ_{MIRS} and also estimates γ of individual litter types. Beside the open questions mentioned in the previous subsection, we suggest that this model can be extended to incorporate additional information. For example, we did not incorporate prior information on differences in decomposition rates between litter types and this may lead to more accurate estimates for γ. A natural extension of the mixing model is to link it to a process model that constrains γ of individual litter types.

Overall, this evaluation suggests that γ_{MIRS} fulfills many properties of an ideal decomposition indicator, even if not applicable to all peat samples. Despite many opportunities for improvements, we are not aware of a decomposition indicator that has the potential to predict γ as well as does γ_{MIRS} and that can be as easily measured, even with small sample amounts, as is the case for γ_{MIRS}.

4.3 Implications for peatland research and peatland restoration

Here, we discuss some problems in peatland research and restoration that may be addressed with γ_{MIRS} and illustrate some of these points with our analysis of the three mountain bog cores.

1. **Estimation of long-term decomposition rates and improvement of process models**: Our analysis of the peat cores suggests a quite large variation in γ for hummock *Sphagnum* species, with several peaks across the entire depth, even if the peat is several thousands of years old. These differences were probably caused by differences in aerobic decomposition losses since catotelm decomposition rates are assumed to vary less with depth and over time and since at least some layers with larger hummock *Sphagnum* γ coincide with or precede WTD peaks (Fig. 4) (Morris et al., 2015b). Preservation of such variations in peat may allow to better estimate long-term decomposition rates of plant functional types and reconstruct past environmental conditions with process models.

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It is interesting that a small γ (smaller than 50%, median values smaller than 25%) is suggested by all three models (even model 3 that may overestimate γ, Fig. 4) for hummock *Sphagnum* litter in some of the peat samples several hundreds or even thousands of years old and from all three peat cores. Some studies suggest much larger figures for γ (Clymo, 1984; Shao et al., 2022), whereas other studies suggest values for γ similar to those found here (Young et al., 2017; Ramirez et al., 2023). A litterbag synthesis suggests that under aerobic conditions, *S. fuscum* may lose 50% of its initial mass after 20 to 50 years (Teickner et al., 2025d). Assuming a catotelm decomposition rate of 0.0004 yr^{-1}, this would lead to an additional mass loss of ca. 15% over 1000 years and thus a mass loss ca. 20% larger than the upper 90% confidence interval of γ predicted for these samples. This may suggest either that litterbag experiments overestimate decomposition rates (at least under these conditions), that the time until incorporation into the catotelm was even shorter than 20 to 50 years, or that other factors than moisture limited decomposition during these periods (e.g., thermodynamic constraints in the catotelm (e.g., Beer and Blodau, 2007; Blodau et al., 2011), colder temperatures, etc.). When linked to process models, γ_{MIRS} may help to address these questions and therefore to better understand long-term decomposition losses.
Other open problems that may be addressed with γ_{MIRS} are: (1) A more precise quantification of differences in decomposition rates between litter types. If (aboveground) litter from the same layer decomposed under the same environmental conditions, current decomposition models (e.g., Frolking et al., 2001) assume that differences in γ rates are only controlled by differences in the maximum possible decomposition rates of these litter types. This allows to estimate differences or ratios of litter type-specific decomposition rates from γ_{MIRS} of individual litter types (supporting information S4). (2) It is commonly assumed that decomposition rates slow down the more of the initial mass has already been decomposed and this is an important control of long-term peat accumulation rates (e.g. Frolking et al., 2001; Clymo et al., 1998). However, this slow-down is difficult to quantify (Frolking et al., 2001; Clymo et al., 1998) because the effect only manifests over long time periods not covered by litterbag experiments and because of difficulties to accurately estimate decomposition parameters from peat cores; measurements of γ_{MIRS} from many peat cores and samples across large time gradients may help to address this problem (supporting information S4). (3) Similarly to the slow-down due to decreasing litter quality, it is assumed that anaerobic decomposition rates decrease with depth due to thermodynamic limitations (e.g., Beer and Blodau, 2007; Blodau et al., 2011), which can have large effects on long-term peat accumulation (Quillet et al., 2013). Measurements of γ_{MIRS} may complement targeted litterbag experiments to better estimate this decrease in anaerobic decomposition rates (Teickner et al., 2025d; Frolking et al., 2010).

2. **Analysis of the WTD-decomposition feedback**: Saturated hydraulic conductivity (K_{sat}) is an important control of peatland WTD and depends on the pore size distribution which in turn depends on the stiffness of the organic matter (e.g., Mahdiyasa et al., 2022). Decomposition decreases the stiffness and therefore facilitates pore collapse, implying that K_{sat} and γ are negatively related (e.g., Morris et al., 2011). Several studies hypothesized relations between saturated hydraulic conductivity (K_{sat}) and γ (Frolking et al., 2010, with corrected formulas as included in the supplement to Treat et al. (2022); Morris et al., 2011; Morris et al., 2015a; Mahdiyasa et al., 2022; Mahdiyasa et al., 2023), but these hypotheses could only be evaluated against not well tested proxies of γ, such as ratios of C/N values (Morris et al.,

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2015a), if at all. To test these hypotheses, we predicted K_{sat} for the peat samples analyzed here from MIRS and plotted these predictions versus γ together with the suggested K_{sat}-γ relations (Fig. 5). The results indicate that, at least for the cores analyzed here, default parameterizations differ from estimated averages (albeit one has to consider that both K_{sat} and γ estimates have relatively large errors). Estimation of γ from peat MIRS would also allow to test the relation between γ and Young's modulus suggested in Mahdiyasa et al. (2022) and Mahdiyasa et al. (2023), and thus also the suggested relations to porosity, bulk density, and K_{sat} suggested therein, if measurements for Young's modulus of peat would be available. Our analysis indicates that γ_{MIRS} may be useful to estimate processes relevant to better understand the ecohydrological feedback in peatlands and to improve existing peatland models.

3. **Definition of reference states for restoration and long-term monitoring of peatland states**: Peatland restoration usually aims to restore the peat accumulation function by increasing NPP and reducing decomposition losses. Here, γ_{MIRS} can be useful to define baselines for the NPP of individual species and the overall NPP, and what fraction of the initial mass should be transferred from the acrotelm to the catotelm. For example, based on our results, one may target a NPP of ca. 0.2 kg m^{-1} yr^{-1} at MH1 as historical reference state for restoration since this corresponds to the past average NPP over several centuries where the small γ indicates that much of this sequestered C is stored in the catotelm. Our analysis also suggests that a drying trend during the last decades halved the NPP (Fig. 4). Here, γ_{MIRS} allows to distinguish between a reduction in NPP versus an increase in decomposition losses. While a process model analysis is necessary to estimate net mass or carbon balances (Young et al., 2021), a decrease in NPP and increase in γ of surface peat very likely indicate a decrease in the net mass or carbon balance since the acrotelm contributes most to decomposition losses. Considering that no long-term measurements of gas fluxes are required to obtain this information, but only standard analyses of peat cores, this may be a cost-efficient approach to estimate how much the current state of a peatland differs from more pristine states in the past and to evaluate restoration over longer time periods. Our analysis also illustrates the possibility to define site-specific reference states for NPP of target communities that were realized at the site over long time periods because γ_{MIRS} allows to infer that NPP has probably always been smaller at MK1 and OD2 than at MH1 (Fig. 4). The rather large errors in the reconstruction here can be reduced not only by improving prediction of γ_{MIRS}, but also by more precise dating and by replacing MIRS-predicted bulk densities with bulk density measurements.

   In summary, this suggests that γ_{MIRS} may be useful to better understand peat accumulation, improve process models, define baselines for peatland restoration, and monitor long-term restoration trajectories.

5 Conclusions

To address the question whether it is possible to estimate γ of peat samples, we developed models that predict γ measured in litterbag experiments from MIRS (γ_{MIRS}) and a mixing model that compensates biases in γ_{MIRS} for mixtures of litter types and therefore allows to estimate γ from γ_{MIRS} with bulk MIRS measurements.

Our model evaluation suggests that the models accurately fit γ of several litter types, that the models do not confound differ-

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ences in litter chemistry or additions of minerals with decomposition, and that our mixing model can correct underestimation of γ by γ_{MIRS} for litter mixtures with known mass fraction of each component, which allows to estimate γ of dominant components, to estimate the average γ of the sample, and to reconstruct the aboveground NPP (in absence of roots) of dominant litter types and the entire vegetation community at the sampling location.

As is the case for all novel and complex prediction models, intensive testing is required to address remaining limitations and reduce prediction errors and some of this work remains to be done by future studies. Main limitations are that there is a relatively large variability in median predictions of γ between prediction models using differently preprocessed MIRS due to biases for litter with small N contents (model 1), possible overfitting (model 2 and 3), extrapolation for more decomposed peat samples and therefore larger prediction errors (all models), large prediction errors for mineral-rich samples, missing woody plant organs in the training data, and possible limitations we could not test here (for example the influence of carbonates). Despite these limitations, γ_{MIRS} fulfills many of the properties of an ideal decomposition indicator and is a promising first step towards accurate estimation of peat γ and reconstruction of past NPP, in particular compared to other the ash residue method, which has large errors, and other decomposition indicators, which cannot estimate γ quantitatively.

Our analysis of three mountain bog peat cores illustrates that, if the limitations of the models are considered, γ_{MIRS} may be useful to estimate γ and reconstruct past aboveground NPP for individual litter types and peat samples. We discussed that these estimates of γ may be useful to address a number of questions relevant to understand peatland processes and to plan and monitor peatland restoration (in particular when studies measure MIRS for individual litter types): Estimating long-term rates of peat decomposition, using peat cores as long-term litterbag experiments to understand environmental controls (thermodynamics limitations, decrease of litter quality), testing hypotheses about long-term decomposition processes (e.g., the time taken to incorporate peat into the catotelm), estimating the feedback between decomposition and peat hydraulic properties (e.g., the $K_{\text{sat}} - \gamma$ relation), and definition of past reference states for NPP and decomposition losses. Preliminary results indicate that *Sphagnum* peat can have a small γ even if it is several hundreds to thousands years old, and that at, least for the cores analyzed here, suggested $K_{\text{sat}} - \gamma$ relations differ from the averages estimated here and vary between peat cores.

Thus, γ_{MIRS} may be useful to improve understanding of peat accumulation dynamics, process models, and may be used for a cost-efficient definition of peatland reference states and monitoring restoration trajectories.

Code and data availability. Peat data are available from the pmird database (Teickner et al., 2025a). Litter data are available from the pmird database (undecomposed litter, data from Reuter et al. (2019a) and Reuter et al. (2019b)), and Arsenault et al. (2024b) (all data except spectra, which are available from Teickner et al. (2025b)). The code to reproduce this manuscript and the mid-infrared spectra for samples in Arsenault et al. (2024b) are available from Teickner et al. (2025b). An R-package to estimate the mixing model for peat samples is available from Teickner (2025b).

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https://doi.org/10.5194/egusphere-2025-5819
Preprint. Discussion started: 23 December 2025

References

Agethen, S. and Knorr, K.-H.: *Juncus Effusus* Mono-Stands in Restored Cutover Peat Bogs – Analysis of Litter Quality, Controls of Anaerobic Decomposition, and the Risk of Secondary Carbon Loss, Soil Biology and Biochemistry, 117, 139–152, https://doi.org/10.1016/j.soilbio.2017.11.020, 2018.

Anzenhofer, R.: Biogeochemical Characterization of Peat Profiles along a Vegetation Gradient in an Ombrotrophic Bog, Patagonia, Master's thesis, 2014, unpublished.

Arsenault, J., Talbot, J., Moore, T. R., Knorr, K.-H., Teickner, H., and Lapierre, J.-F.: Patterns and Drivers of Organic Matter Decomposition in Peatland Open-Water Pools, Biogeosciences, 21, 3491–3507, https://doi.org/10.5194/bg-21-3491-2024, 2024a.

Arsenault, J., Talbot, J., Moore, T. R., Knorr, K.-H., Teickner, H., and Lapierre, J.-F.: Patterns and Drivers of Organic Matter Decomposition in Peatland Open-Water Pools, https://doi.org/10.5281/ZENODO.10581235, 2024b.

Artz, R. R., Chapman, S. J., Jean Robertson, A., Potts, J. M., Laggoun-Défarge, F., Gogo, S., Comont, L., Disnar, J.-R., and Francez, A.-J.: FTIR Spectroscopy Can Be Used as a Screening Tool for Organic Matter Quality in Regenerating Cutover Peatlands, Soil Biology and Biochemistry, 40, 515–527, https://doi.org/10.1016/j.soilbio.2007.09.019, 2008.

Bauer, I. E.: Modelling Effects of Litter Quality and Environment on Peat Accumulation over Different Time-Scales: Peat Accumulation over Different Time-Scales, Journal of Ecology, 92, 661–674, https://doi.org/10.1111/j.0022-0477.2004.00905.x, 2004.

Beer, J. and Blodau, C.: Transport and Thermodynamics Constrain Belowground Carbon Turnover in a Northern Peatland, Geochimica et Cosmochimica Acta, 71, 2989–3002, https://doi.org/10.1016/j.gca.2007.03.010, 2007.

Beleites, C. and Sergo, V.: hyperSpec: A Package to Handle Hyperspectral Data Sets in R, 2021.

Belyea, L. R. and Baird, A. J.: Beyond "The Limits to Peat Bog Growth": Cross-Scale Feedback in Peatland Developent, Ecological Monographs, 76, 299–322, https://doi.org/10.1890/0012-9615(2006)076[0299:BTLTPB]2.0.CO;2, 2006.

Bengtsson, F., Rydin, H., Baltzer, J., Bragazza, L., Bu, Z.-J., Caporn, S., Dorrepaal, E., Flatberg, K. I., Galanina, O., Gałka, M., Ganeva, A., Goia, I., Goncharova, N., Hajek, M., Haraguchi, A., Harris, L., Humphreys, E., Jiroušek, M., Kajukało, K., Karofeld, E., Koronatova, N., Kosykh, N., Laine, A., Lamentowicz, M., Lapshina, E., Limpens, J., Linkosalmi, M., Ma, J., Mauritz, M., Mitchell, E., Munir, T., Natali, S., Natcheva, R., Philippov, D., Rice, S., Robinson, S., Robroek, B., Rochefort, L., Singer, D., Stenøien, H., Tuittila, E.-S., Vellak, K., Waddington, J. M., Granath, G., and Payne, R. J.: Environmental Drivers of *Sphagnum* Growth in Peatlands across the Holarctic Region, https://doi.org/10.5061/DRYAD.1NS1RN8RM, 2020.

Bengtsson, F., Rydin, H., Baltzer, J. L., Bragazza, L., Bu, Z.-J., Caporn, S. J. M., Dorrepaal, E., Flatberg, K. I., Galanina, O., Gałka, M., Ganeva, A., Goia, I., Goncharova, N., Hájek, M., Haraguchi, A., Harris, L. I., Humphreys, E., Jiroušek, M., Kajukało, K., Karofeld, E., Koronatova, N. G., Kosykh, N. P., Laine, A. M., Lamentowicz, M., Lapshina, E., Limpens, J., Linkosalmi, M., Ma, J.-Z., Mauritz, M., Mitchell, E. A. D., Munir, T. M., Natali, S. M., Natcheva, R., Payne, R. J., Philippov, D. A., Rice, S. K., Robinson, S., Robroek, B. J. M., Rochefort, L., Singer, D., Stenøien, H. K., Tuittila, E.-S., Vellak, K., Waddington, J. M., and Granath, G.: Environmental Drivers of *Sphagnum* Growth in Peatlands across the Holarctic Region, Journal of Ecology, 109, 417–431, https://doi.org/10.1111/1365-2745.13499, 2021.

Biester, H., Knorr, K.-H., Schellekens, J., Basler, A., and Hermanns, Y.-M.: Comparison of Different Methods to Determine the Degree of Peat Decomposition in Peat Bogs, Biogeosciences, 11, 2691–2707, https://doi.org/10.5194/bg-11-2691-2014, 2014.

Blaauw, M., Christen, J. A., and Aquino Lopez, M. A.: rbacon: Age-depth Modelling Using Bayesian Statistics, https://doi.org/10.32614/CRAN.package.rbacon, 2017.

https://doi.org/10.5194/egusphere-2025-5819
Preprint. Discussion started: 23 December 2025

Blodau, C., Siems, M., and Beer, J.: Experimental Burial Inhibits Methanogenesis and Anaerobic Decomposition in Water-Saturated Peats, Environmental Science & Technology, 45, 9984–9989, https://doi.org/10.1021/es201777u, 2011.

Bona, K. A., Hilger, A., Burgess, M., Wozney, N., and Shaw, C.: A Peatland Productivity and Decomposition Parameter Database, Ecology, 99, 2406–2406, https://doi.org/10.1002/ecy.2462, 2018.

Boothroyd, I. M., Worrall, F., Moody, C. S., Clay, G. D., Abbott, G. D., and Rose, R.: Sulfur Constraints on the Carbon Cycle of a Blanket Bog Peatland, Journal of Geophysical Research: Biogeosciences, 126, https://doi.org/10.1029/2021JG006435, 2021.

Broder, T., Blodau, C., Biester, H., and Knorr, K. H.: Peat Decomposition Records in Three Pristine Ombrotrophic Bogs in Southern Patagonia, Biogeosciences, 9, 1479–1491, https://doi.org/10.5194/bg-9-1479-2012, 2012.

Bürkner, P.-C.: Advanced Bayesian Multilevel Modeling with the R Package brms, The R Journal, 10, 395–411, https://doi.org/10.32614/RJ-2018-017, 2018.

Chapman, S., Campbell, C., Fraser, A., and Puri, G.: FTIR Spectroscopy of Peat in and Bordering Scots Pine Woodland: Relationship with Chemical and Biological Properties, Soil Biology and Biochemistry, 33, 1193–1200, https://doi.org/10.1016/S0038-0717(01)00023-2, 2001.

Clymo, R. S.: The Limits to Peat Bog Growth, Philosophical transactions of the Royal Society of London. Series B, Biological sciences, 303, 51, 1984.

Clymo, R. S., Turunen, J., and Tolonen, K.: Carbon Accumulation in Peatland, Oikos, 81, 368–388, https://doi.org/10.2307/3547057, 1998.

Cocozza, C., D'Orazio, V., Miano, T. M., and Shotyk, W.: Characterization of Solid and Aqueous Phases of a Peat Bog Profile Using Molecular Fluorescence Spectroscopy, ESR and FT-IR, and Comparison with Physical Properties, Organic Geochemistry, 34, 49–60, https://doi.org/10.1016/S0146-6380(02)00208-5, 2003.

Cotrufo, M. F. and Pressler, Y.: Isotope Mixing, pp. 53–70, Oxford University PressOxford, 1 edn., ISBN 978-0-19-885449-4 978-0-19-188878-6, https://doi.org/10.1093/oso/9780198854494.003.0004, 2023.

Diaconu, A.-C., Tanţău, I., Knorr, K.-H., Borken, W., Feurdean, A., Panait, A., and Gałka, M.: A Multi-Proxy Analysis of Hydroclimate Trends in an Ombrotrophic Bog over the Last Millennium in the Eastern Carpathians of Romania, Palaeogeography, Palaeoclimatology, Palaeoecology, 538, 109 390, https://doi.org/10.1016/j.palaeo.2019.109390, 2020.

Drollinger, S., Kuzyakov, Y., and Glatzel, S.: Effects of Peat Decomposition on δ^{13}C and δ^{15}N Depth Profiles of Alpine Bogs, CATENA, 178, 1–10, https://doi.org/10.1016/j.catena.2019.02.027, 2019.

Drollinger, S., Knorr, K.-H., Knierzinger, W., and Glatzel, S.: Peat Decomposition Proxies of Alpine Bogs along a Degradation Gradient, Geoderma, 369, 114 331, https://doi.org/10.1016/j.geoderma.2020.114331, 2020.

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.

Frolking, S., Roulet, N. T., Moore, T. R., Richard, P. J. H., Lavoie, M., and Muller, S. D.: Modeling Northern Peatland Decomposition and Peat Accumulation, Ecosystems, 4, 479–498, https://doi.org/10.1007/s10021-001-0105-1, 2001.

Frolking, S., Roulet, N. T., Tuittila, E., Bubier, J. L., Quillet, A., Talbot, J., and Richard, P. J. H.: A New Model of Holocene Peatland Net Primary Production, Decomposition, Water Balance, and Peat Accumulation, Earth System Dynamics, 1, 1–21, https://doi.org/10.5194/esd-1-1-2010, 2010.

Gałka, M., Diaconu, A.-C., Feurdean, A., Loisel, J., Teickner, H., Broder, T., and Knorr, K.-H.: Relations of Fire, Palaeohydrology, Vegetation Succession, and Carbon Accumulation, as Reconstructed from a Mountain Bog in the Harz Mountains (Germany) during the Last 6200 Years, Geoderma, 424, 115 991, https://doi.org/10.1016/j.geoderma.2022.115991, 2022a.

https://doi.org/10.5194/egusphere-2025-5819
Preprint. Discussion started: 23 December 2025

Gałka, M., Hölzer, A., Feurdean, A., Loisel, J., Teickner, H., Diaconu, A.-C., Szal, M., Broder, T., and Knorr, K.-H.: Insight into the Factors of Mountain Bog and Forest Development in the Schwarzwald Mts.: Implications for Ecological Restoration, Ecological Indicators, 140, 109 039, https://doi.org/10.1016/j.ecolind.2022.109039, 2022b.

Hömberg, A.: Geochemische Charakterisierung von Mooren der Changbai Mountains, Bachelor thesis, Münster, Münster, 2014.

Krüger, J. P., Alewell, C., Minkkinen, K., Szidat, S., and Leifeld, J.: Calculating Carbon Changes in Peat Soils Drained for Forestry with Four Different Profile-Based Methods, Forest Ecology and Management, 381, 29–36, https://doi.org/10.1016/j.foreco.2016.09.006, 2016.

Leifeld, J., Gubler, L., and Grünig, A.: Organic Matter Losses from Temperate Ombrotrophic Peatlands: An Evaluation of the Ash Residue Method, Plant and Soil, 341, 349–361, https://doi.org/10.1007/s11104-010-0649-y, 2011a.

Leifeld, J., Müller, M., and Fuhrer, J.: Peatland Subsidence and Carbon Loss from Drained Temperate Fens, Soil Use and Management, 27, 170–176, https://doi.org/10.1111/j.1475-2743.2011.00327.x, 2011b.

Limpens, J. and Berendse, F.: How Litter Quality Affects Mass Loss and N Loss from Decomposing *Sphagnum*, Oikos, 103, 537–547, https://doi.org/10.1034/j.1600-0706.2003.12707.x, 2003.

Loisel, J., Yu, Z., Beilman, D. W., Camill, P., Alm, J., Amesbury, M. J., Anderson, D., Andersson, S., Bochicchio, C., Barber, K., Belyea, L. R., Bunbury, J., Chambers, F. M., Charman, D. J., De Vleeschouwer, F., Fiałkiewicz-Kozieł, B., Finkelstein, S. A., Gałka, M., Garneau, M., Hammarlund, D., Hinchcliffe, W., Holmquist, J., Hughes, P., Jones, M. C., Klein, E. S., Kokfelt, U., Korhola, A., Kuhry, P., Lamarre, A., Lamentowicz, M., Large, D., Lavoie, M., MacDonald, G., Magnan, G., Mäkilä, M., Mallon, G., Mathijssen, P., Mauquoy, D., McCarroll, J., Moore, T. R., Nichols, J., O'Reilly, B., Oksanen, P., Packalen, M., Peteet, D., Richard, P. J., Robinson, S., Ronkainen, T., Rundgren, M., Sannel, A. B. K., Tarnocai, C., Thom, T., Tuittila, E.-S., Turetsky, M., Väliranta, M., van der Linden, M., van Geel, B., van Bellen, S., Vitt, D., Zhao, Y., and Zhou, W.: A Database and Synthesis of Northern Peatland Soil Properties and Holocene Carbon and Nitrogen Accumulation, The Holocene, 24, 1028–1042, https://doi.org/10.1177/0959683614538073, 2014.

Mahdiyasa, A. W., Large, D. J., Muljadi, B. P., Icardi, M., and Triantafyllou, S.: MPeat—A Fully Coupled Mechanical-ecohydrological Model of Peatland Development, Ecohydrology, 15, https://doi.org/10.1002/eco.2361, 2022.

Mahdiyasa, A. W., Large, D. J., Muljadi, B. P., and Icardi, M.: Modelling the Influence of Mechanical-Ecohydrological Feedback on the Nonlinear Dynamics of Peatlands, Ecological Modelling, 478, 110 299, https://doi.org/10.1016/j.ecolmodel.2023.110299, 2023.

Mathijssen, P. J., Gałka, M., Borken, W., and Knorr, K.-H.: Plant Communities Control Long Term Carbon Accumulation and Biogeochemical Gradients in a Patagonian Bog, Science of The Total Environment, 684, 670–681, https://doi.org/10.1016/j.scitotenv.2019.05.310, 2019.

Moore, T. R.: Growth and Net Production of *Sphagnum* at Five Fen Sites, Subarctic Eastern Canada, Canadian Journal of Botany, 67, 1203–1207, https://doi.org/10.1139/b89-156, 1989.

Moore, T. R., Knorr, K.-H., Thompson, L., Roy, C., and Bubier, J. L.: The Effect of Long-Term Fertilization on Peat in an Ombrotrophic Bog, Geoderma, 343, 176–186, https://doi.org/10.1016/j.geoderma.2019.02.034, 2019.

Morris, P. J., Belyea, L. R., and Baird, A. J.: Ecohydrological Feedbacks in Peatland Development: A Theoretical Modelling Study, Journal of Ecology, 99, 1190–1201, https://doi.org/10.1111/j.1365-2745.2011.01842.x, 2011.

Morris, P. J., Baird, A. J., and Belyea, L. R.: The DigiBog Peatland Development Model 2: Ecohydrological Simulations in 2D, Ecohydrology, 5, 256–268, https://doi.org/10.1002/eco.229, 2012.

Morris, P. J., Baird, A. J., and Belyea, L. R.: Bridging the Gap between Models and Measurements of Peat Hydraulic Conductivity, Water Resources Research, 51, 5353–5364, https://doi.org/10.1002/2015WR017264, 2015a.

https://doi.org/10.5194/egusphere-2025-5819
Preprint. Discussion started: 23 December 2025

Morris, P. J., Baird, A. J., Young, D. M., and Swindles, G. T.: Untangling Climate Signals from Autogenic Changes in Long-Term Peatland Development, Geophysical Research Letters, 42, 10,788–10,797, https://doi.org/10.1002/2015GL066824, 2015b.

Parikh, S. J., Goyne, K. W., Margenot, A. J., Mukome, F. N., and Calderón, F. J.: Soil Chemical Insights Provided through Vibrational Spectroscopy, in: Advances in Agronomy, vol. 126, pp. 1–148, Elsevier, ISBN 978-0-12-800132-5, https://doi.org/10.1016/B978-0-12-800132-5.00001-8, 2014.

Piironen, J. and Vehtari, A.: Sparsity Information and Regularization in the Horseshoe and Other Shrinkage Priors, Electronic Journal of Statistics, 11, https://doi.org/10.1214/17-EJS1337SI, 2017a.

Piironen, J. and Vehtari, A.: On the Hyperprior Choice for the Global Shrinkage Parameter in the Horseshoe Prior, arXiv:1610.05559 [stat], 2017b.

Quillet, A., Frolking, S., Garneau, M., Talbot, J., and Peng, C.: Assessing the Role of Parameter Interactions in the Sensitivity Analysis of a Model of Peatland Dynamics, Ecological Modelling, 248, 30–40, https://doi.org/10.1016/j.ecolmodel.2012.08.023, 2013.

Quillet, A., Garneau, M., Van Bellen, S., Frolking, S., and Tuittila, E.-S.: Integration of Palaeohydrological Proxies into a Peatland Model: A New Tool for Palaeoecological Studies, Ecohydrology, 8, 214–229, https://doi.org/10.1002/eco.1501, 2015.

Ramirez, J. A., Peleg, N., Baird, A. J., Young, D. M., Morris, P. J., Larocque, M., and Garneau, M.: Modelling Peatland Development in High-Boreal Quebec, Canada, with DigiBog_Boreal, Ecological Modelling, 478, 110 298, https://doi.org/10.1016/j.ecolmodel.2023.110298, 2023.

Reader, R. J. and Stewart, J. M.: The Relationship between Net Primary Production and Accumulation for a Peatland in Southeastern Manitoba, Ecology, 53, 1024–1037, https://doi.org/10.2307/1935415, 1972.

Reuter, H., Gensel, J., Elvert, M., and Zak, D.: Infrared Spectra (FTIR) of *Phragmites Australis* Litter, Initial and after Anoxic Decomposition in Three Wetland Substrates, https://doi.org/10.1594/PANGAEA.902069, 2019a.

Reuter, H., Gensel, J., Elvert, M., and Zak, D.: CuO Lignin, and Bulk Decomposition Data of a 75-Day Anoxic *Phragmites Australis* Litter Decomposition Experiment in Soil Substrates from Three Northeast German Wetlands, https://doi.org/10.1594/PANGAEA.902176, 2019b.

Reuter, H., Gensel, J., Elvert, M., and Zak, D.: Evidence for Preferential Protein Depolymerization in Wetland Soils in Response to External Nitrogen Availability Provided by a Novel FTIR Routine, Biogeosciences, 17, 499–514, https://doi.org/10.5194/bg-17-499-2020, 2020.

Rochefort, L., Vitt, D. H., and Bayley, S. E.: Growth, Production, and Decomposition Dynamics of *Sphagnum* under Natural and Experimentally Acidified Conditions, Ecology, 71, 1986–2000, https://doi.org/10.2307/1937607, 1990.

Scheffer, R. A., Van Logtestijn, R. S. P., and Verhoeven, J. T. A.: Decomposition of *Carex* and *Sphagnum* Litter in Two Mesotrophic Fens Differing in Dominant Plant Species, Oikos, 92, 44–54, https://doi.org/10.1034/j.1600-0706.2001.920106.x, 2001.

Shao, S., Wu, J., He, H., and Roulet, N.: Integrating McGill Wetland Model (MWM) with Peat Cohort Tracking and Microbial Controls, Science of The Total Environment, 806, 151 223, https://doi.org/10.1016/j.scitotenv.2021.151223, 2022.

Sivula, T., Magnusson, M., Matamoros, A. A., and Vehtari, A.: Uncertainty in Bayesian Leave-One-out Cross-Validation Based Model Comparison, https://doi.org/10.48550/arXiv.2008.10296, 2022.

Stan Development Team: Stan Modeling Language Users Guide and Reference Manual, 2021.

Stuart, B. H.: Infrared Spectroscopy: Fundamentals and Applications, Analytical Techniques in the Sciences, John Wiley & Sons, Ltd, Chichester, UK, ISBN 978-0-470-01114-0 978-0-470-85428-0, https://doi.org/10.1002/0470011149, 2004.

Szumigalski, A. R.: Production and Decomposition of Vegetation along a Wetland Gradient in Central Alberta, https://doi.org/10.7939/R3B27PW45, 1995.

https://doi.org/10.5194/egusphere-2025-5819
Preprint. Discussion started: 23 December 2025

Tatzber, M., Stemmer, M., Spiegel, H., Katzlberger, C., Haberhauer, G., and Gerzabek, M. H.: An Alternative Method to Measure Carbonate in Soils by FT-IR Spectroscopy, Environmental Chemistry Letters, 5, 9–12, https://doi.org/10.1007/s10311-006-0079-5, 2007.

Teickner, H.: ir: Functions to Handle and Preprocess Infrared Spectra, https://doi.org/10.32614/CRAN.package.ir, 2022.

Teickner, H.: irpeatmodels: Mid-infrared Prediction Models for Peat, Zenodo, https://doi.org/10.5281/ZENODO.17187912, 2025a.

Teickner, H.: mmgm: Estimates the Degree of Decomposition of Peat with a Mixing Model for γ_{MIRS}, Zenodo, https://doi.org/10.5281/ZENODO.17209338, 2025b.

Teickner, H. and Knorr, K.-H.: Improving Models to Predict Holocellulose and Klason Lignin Contents for Peat Soil Organic Matter with Mid-Infrared Spectra, SOIL, 8, 699–715, https://doi.org/10.5194/soil-8-699-2022, 2022.

Teickner, H. and Knorr, K.-H.: Prediction of Peat Properties from Transmission Mid-Infrared Spectra, https://doi.org/10.5194/egusphere-2025-4955, 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., 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, 2025a.

Teickner, H., Arsenault, J., Galka, M., and Knorr, K.-H.: Compendium of R Code and Data for "Estimation of the Degree of Decomposition of Peat and Past Net Primary Production from Mid-Infrared Spectra", Zenodo, https://doi.org/10.5281/ZENODO.17209547, 2025b.

Teickner, H., Pebesma, E., and Knorr, K.-H.: A Synthesis of *Sphagnum* Litterbag Experiments: Initial Leaching Losses Bias Decomposition Rate Estimates, Biogeosciences, 22, 417–433, https://doi.org/10.5194/bg-22-417-2025, 2025c.

Teickner, H., Pebesma, E., and Knorr, K.-H.: Peat Oxic and Anoxic Controls of *Sphagnum* Decomposition Rates in the Holocene Peatland Model Decomposition Module Estimated from Litterbag Data, Earth System Dynamics, 16, 891–914, https://doi.org/10.5194/esd-16-891-2025, 2025d.

Tfaily, M. M., Cooper, W. T., Kostka, J. E., Chanton, P. R., Schadt, C. W., Hanson, P. J., Iversen, C. M., and Chanton, J. P.: Organic Matter Transformation in the Peat Column at Marcell Experimental Forest: Humification and Vertical Stratification: Organic Matter Dynamics, Journal of Geophysical Research: Biogeosciences, 119, 661–675, https://doi.org/10.1002/2013JG002492, 2014.

Thormann, M. N. and Bayley, S. E.: Aboveground Net Primary Production along a Bog-Fen-Marsh Gradient in Southern Boreal Alberta, Canada, Écoscience, 4, 374–384, https://doi.org/10.1080/11956860.1997.11682416, 1997.

Treat, C. C., Jones, M. C., Alder, J., and Frolking, S.: Hydrologic Controls on Peat Permafrost and Carbon Processes: New Insights from Past and Future Modeling, Frontiers in Environmental Science, 10, 892 925, https://doi.org/10.3389/fenvs.2022.892925, 2022.

Tuittila, E.-S., Juutinen, S., Frolking, S., Väliranta, M., Laine, A. M., Miettinen, A., Seväkivi, M.-L., Quillet, A., and Merilä, P.: Wetland Chronosequence as a Model of Peatland Development: Vegetation Succession, Peat and Carbon Accumulation, The Holocene, 23, 25–35, https://doi.org/10.1177/0959683612450197, 2013.

Vehtari, A., Gabry, J., Magnusson, M., Yao, Y., Bürkner, P.-C., Paananen, T., Gelman, A., Goodrich, B., and Piironen, J.: loo: Efficient Leave-One-out Cross-Validation and WAIC for Bayesian Models, 2019.

Vehtari, A., Gelman, A., Simpson, D., Carpenter, B., and Bürkner, P.-C.: Rank-Normalization, Folding, and Localization: An Improved R^ for Assessing Convergence of MCMC (with Discussion), Bayesian Analysis, 16, 667–718, https://doi.org/10.1214/20-BA1221, 2021.

https://doi.org/10.5194/egusphere-2025-5819
Preprint. Discussion started: 23 December 2025

Viscarra Rossel, R. A., Shen, Z., Ramirez Lopez, L., Behrens, T., Shi, Z., Wetterlind, J., Sudduth, K. A., Stenberg, B., Guerrero, C., Gholizadeh, A., Ben-Dor, E., St Luce, M., and Orellano, C.: An Imperative for Soil Spectroscopic Modelling Is to Think Global but Fit Local with Transfer Learning, Earth-Science Reviews, 254, 104 797, https://doi.org/10.1016/j.earscirev.2024.104797, 2024.

Waddington, J. M., Morris, P. J., Kettridge, N., Granath, G., Thompson, D. K., and Moore, P. A.: Hydrological Feedbacks in Northern Peatlands, Ecohydrology, 8, 113–127, https://doi.org/10.1002/eco.1493, 2015.

Wadoux, A. M.-C., Malone, B., Minasny, B., Fajardo, M., and McBratney, A. B.: Soil Spectral Inference with R: Analysing Digital Soil Spectra Using the R Programming Environment, Progress in Soil Science, Springer International Publishing, Cham, ISBN 978-3-030-64896-1, https://doi.org/10.1007/978-3-030-64896-1, 2021.

Wagner, S.: Analysis of Peat Decomposition, Element Distribution Patterns and Element Output of Two Peat Bogs in the Thuringian Forest, Master's thesis, University Bayreuth, 2013.

Wallace, W. E. and NIST Mass Spectrometry Data Center: Infrared Spectra, in: NIST Chemistry WebBook, NIST Standard Reference Database 69, National Institute of Standards and Technology, Gaithersburg MD, 20899, 1997.

Wieder, R. K., Vile, M. A., Albright, C. M., Scott, K. D., Vitt, D. H., Quinn, J. C., and Burke-Scoll, M.: Effects of Altered Atmospheric Nutrient Deposition from Alberta Oil Sands Development on *Sphagnum Fuscum* Growth and C, N and S Accumulation in Peat, Biogeochemistry, 129, 1–19, https://doi.org/10.1007/s10533-016-0216-6, 2016.

Wieder, R. K., Vitt, D. H., Vile, M. A., Graham, J. A., Hartsock, J. A., Fillingim, H., House, M., Quinn, J. C., Scott, K. D., Petix, M., and McMillen, K. J.: Experimental Nitrogen Addition Alters Structure and Function of a Boreal Bog: Critical Load and Thresholds Revealed, Ecological Monographs, 89, https://doi.org/10.1002/ecm.1371, 2019.

Worrall, F.: Sulphur Constraints on the Carbon Cycle of a Blanket Bog Peatland [Dataset], https://doi.org/10.15128/R2PK02C9794, 2021.

Young, D. M., Baird, A. J., Morris, P. J., and Holden, J.: Simulating the Long-term Impacts of Drainage and Restoration on the Ecohydrology of Peatlands, Water Resources Research, 53, 6510–6522, https://doi.org/10.1002/2016WR019898, 2017.

Young, D. M., Baird, A. J., Gallego-Sala, A. V., and Loisel, J.: A Cautionary Tale about Using the Apparent Carbon Accumulation Rate (aCAR) Obtained from Peat Cores, Scientific Reports, 11, 9547, https://doi.org/10.1038/s41598-021-88766-8, 2021.

Zaccone, C., Plaza, C., Ciavatta, C., Miano, T. M., and Shotyk, W.: Advances in the Determination of Humification Degree in Peat since Achard (1786): Applications in Geochemical and Paleoenvironmental Studies, Earth-Science Reviews, 185, 163–178, https://doi.org/10.1016/j.earscirev.2018.05.017, 2018.