Supplement of Earth Syst. Dynam., 16, 891–914, 2025
https://doi.org/10.5194/esd-16-891-2025-supplement

Supplement of

Peat oxic and anoxic controls of *Sphagnum* decomposition rates in the Holocene Peatland Model decomposition module estimated from litterbag data

Henning Teickner et al.

Correspondence to: Henning Teickner (henning.teickner@uni-muenster.de)

Contents

S1 Prior choices and justification

Table S1: Prior distributions of all Bayesian models and their justifications. “Parameter name in code” is the name for the parameter as used in our Stan models. “Parameter name in text” is the name of the corresponding parameter we use in the main text and figures. “Equation in main text” references the equation in the main text where the parameter occurs. When there is no value for “Justification”, the prior was chosen based on prior predictive checks against the data. This prior predictive check tests whether the models can produce distributions of measured variables we expect based on prior knowledge. The results of these prior predictive checks are shown in supporting section S3.

Parameter name in code	Parameter name in text	Equation in main text	Unit	Prior distribution	Justification
l_2_p1			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	normal(-3.5, l_2_p1_p2)	Assumes an average initial leaching loss across all available litterbag data within (95% confidence interval) (0.012, 0.068) g $\mathrm{g}_{\mathrm{initial}}^{-1}$
l_2_p2			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	normal(0, l_2_p2_p2)	
l_2_p3			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	normal(0, l_2_p3_p2)	
l_2_p4			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	normal(0, l_2_p4_p2)	
k_2_p1	$\beta_{k,1}$	4	(yr^{-1}) (log scale)	normal(-2.9, k_2_p1_p2)	Assumes an average initial decomposition rate across all available litterbag data within (95% confidence interval) (0.024, 0.131) yr^{-1}
k_2_p2	$\beta_{k,2,\mathrm{species}}$	4	(yr^{-1}) (log scale)	normal(0, k_2_p2_p2)	Centered at the standard value used in the HPM.
k_2_p3	$\beta_{k,3,\mathrm{species\ x\ study}}$	4	(yr^{-1}) (log scale)	normal(0, k_2_p3_p2)	Centered at the standard value used in the HPM.
k_2_p4	$\beta_{k,4,\mathrm{sample}}$	4	(yr^{-1}) (log scale)	normal(0, k_2_p4_p2)	Centered at the standard value used in the HPM.
phi_2_p2_p1			(-) (log scale)	normal(5, phi_2_p2_p1_p2)	
phi_2_p2_p2			(-) (log scale)	normal(0, phi_2_p2_p2_p2)	
phi_2_p2_p3			(-) (log scale)	normal(0, phi_2_p2_p3_p2)	
phi_2_p2_p4			(-) (log scale)	normal(0, phi_2_p2_p4_p2)	
alpha_2_p1			(-) (log scale)	normal(-0.2, 0.3)	Assumes an average α across all available litterbag data within (95% confidence interval) (1.451, 2.473)
alpha_2_p2			(-) (log scale)	normal(0, 0.3)	
alpha_2_p3			(-) (log scale)	normal(0, 0.3)	
alpha_2_p4			(-) (log scale)	normal(0, 0.2)	
k_2_p1_p2			(yr^{-1}) (log scale)	half-normal(0, 0.4)	
k_2_p2_p2			(yr^{-1}) (log scale)	half-normal(0, 0.4)	
k_2_p3_p2			(yr^{-1}) (log scale)	half-normal(0, 0.4)	
k_2_p4_p2			(yr^{-1}) (log scale)	half-normal(0, 0.4)	
phi_2_p2_p1_p2			(-) (log scale)	half-normal(0, 0.3)	
phi_2_p2_p2_p2			(-) (log scale)	half-normal(0, 0.3)	
phi_2_p2_p3_p2			(-) (log scale)	half-normal(0, 0.3)	
phi_2_p2_p4_p2			(-) (log scale)	half-normal(0, 0.3)	
l_2_p1_p2			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	half-normal(0, 0.4)	
l_2_p2_p2			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	half-normal(0, 0.4)	
l_2_p3_p2			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	half-normal(0, 0.4)	
l_2_p4_p2			(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	half-normal(0, 0.4)	
layer_total_porosity_1	P	9	$\mathrm{L}_{\mathrm{pores}}\ \mathrm{L}_{\mathrm{sample}}^{-1}$	beta(12, 3)	Centered at the standard value used in the HPM.
layer_minimum_degree_of_saturation_at_surface_1	$\theta_{0,\mathrm{min}}$	9	$\mathrm{L}_{\mathrm{water}}\ \mathrm{L}_{\mathrm{pores}}^{-1}$	beta(0.9, 17.1)	Centered at the standard value used in the HPM.
layer_water_table_depth_to_surface_1			cm	normal(average reported WTD, 3)	The average was set to the average water table depths reported in the litterbag studies.
hpm_k_2_p1	α_{μ_k}	8	(-)	gamma(20, 1)	Centered at the standard value used in the HPM.
m69_p1	W_{opt}	6	$\mathrm{L}_{\mathrm{water}}\ \mathrm{L}_{\mathrm{pores}}^{-1}$	beta(13.5, 16.5)	Centered at the standard value used in the HPM.
m69_p2	c_1	6	(-)	gamma(20, 8.66)	Centered at the standard value used in the HPM.
m68_p1	f_{min}	7	(yr^{-1})	gamma(5, 5000)	Centered at the standard value used in the HPM.
m68_p2	c_2	7	(cm)	gamma(5, 16.67)	Centered at the standard value used in the HPM.
m68_p3_2_p1	$k_{0,i}$	5	(yr^{-1}) (log scale)	normal(-2.2, 0.3)	Assumes a maximum potential initial decomposition rate across all species within (95% confidence interval) (0.061, 0.2) yr^{-1}
hpm_l_2_p1	$\beta_{l,1}$	10	(g $\mathrm{g}_{\mathrm{initial}}^{-1}$) (logit scale)	normal(-2.2, 0.3)	Centered at the standard value used in the HPM.
hpm_l_2_p3	$\beta_{l,2}$	10	(g $\mathrm{g}_{\mathrm{initial}}^{-1}\ \mathrm{L}_{\mathrm{water}}^{-1}\ \mathrm{L}_{\mathrm{pores}}$) (logit scale)	normal(0, 0.5)	Centered at the standard value used in the HPM.
hpm_l_2_p4	ϕ_l	10	(-)	gamma(10, 0.25)	Centered at the standard value used in the HPM.

S2 Further Information on Bayesian Data Analysis

Monte Carlo Standard Errors Monte Carlo standard errors (MSCE) (Vehtari et al., 2021) for the median were at most 0.012 yr^{-1} for k_0, 0.363 mass-% for l_0, 0.043 for α, 0.401 mass-% for the remaining mass, 0.001 $\mathrm{L_{water}\ L_{pores}^{-1}}$ for W_{opt}, 0.004 for c_1, 0.001 yr^{-1} for f_{min}, 0.002 m for c_2, 0.003 yr^{-1} for k_0 predicted by the HPM modifications, and 0.342 mass-% for l_0 predicted by HPM-leaching. For the 2.5% and 97.5% quantiles, MCSE were at most 0.088 yr^{-1} for k_0, 0.646 mass-% for l_0, 0.147 for α, 2.742 mass-% for the remaining mass, 0.004 $\mathrm{L_{water}\ L_{pores}^{-1}}$ for W_{opt}, 0.006 for c_1, 0.005 yr^{-1} for f_{min}, 0.007 m for c_2, 0.003 yr^{-1} for k_0 predicted by the HPM modifications, and 0.293 mass-% for l_0 predicted by HPM-leaching.

Power-scaling Power-scaling exponentiates prior (to analyze prior sensitivity) or likelihood (to analyze likelihood sensitivity) distributions by different constants $\alpha > 0$, where $\alpha > 1$ means that the scaled component gets more important relative to the other component, and $\alpha < 1$ means it gets less important (Kallioinen et al., 2024). We varied α from 0.99 to 1.01 (default option) and identified sensitivity with the cumulative Jensen-Shannon distance and a threshold of 0.05, as suggested in Kallioinen et al. (2024).

The power-scaling sensitivity analysis indicates a weak likelihood for all peat properties for most litterbag experiments, indicating that, not surprisingly, remaining masses alone do not give much information about peat properties. For W_{opt}, c_1, and c_2 the analysis suggested a prior-data conflict which supports our finding that parameter values different from the standard values are more compatible with the data. For $k_{0,i}$, the analysis suggested a prior-data conflict for most species, and similar for the parameters with which we modeled how initial leaching losses depend on the degree of saturation. We did not attempt to resolve these conflicts, either because we know from our previous study that the data provide only uncertain information (Teickner et al., 2025) which makes prior-data conflicts more likely, or because we wanted to use HPM standard parameter values as prior information. A future update of our study with more accurate data may address these challenges.

Software All computations were done in R (4.2.0) (R Core Team, 2022). We computed prior and posterior predictive checks with the bayesplot package (1.9.0) (Gabry and Mahr, 2022) (supporting section S3). Data were handled with tidyverse packages (Wickham et al., 2019), MCMC samples with the posterior (1.5.0) (Bürkner et al., 2023) and tidybayes (3.0.2) (Kay, 2022b) packages. Graphics were created with ggplot2 (3.4.4) (Wickham, 2016), ggdist (3.1.1) (Kay, 2022a) and patchwork (1.1.1) (Pedersen, 2020).

S3 Prior and posterior predictive checks

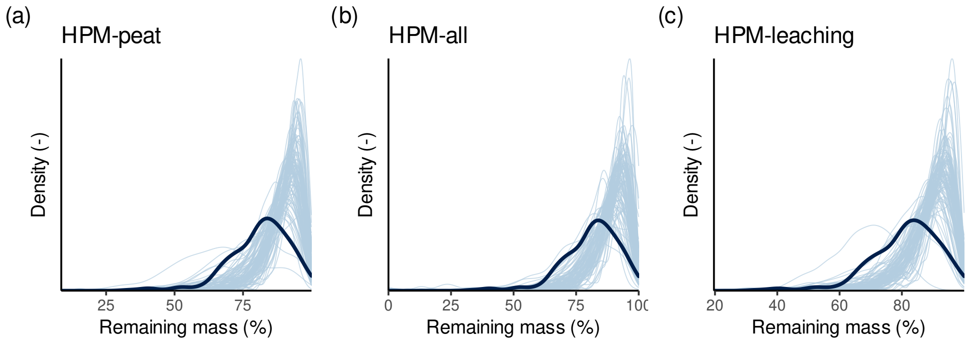


Figure S1: Density estimate of 100 sets of remaining masses sampled from the prior distribution of each model (light blue lines) versus density estimate of the measured remaining masses from the litterbag studies.

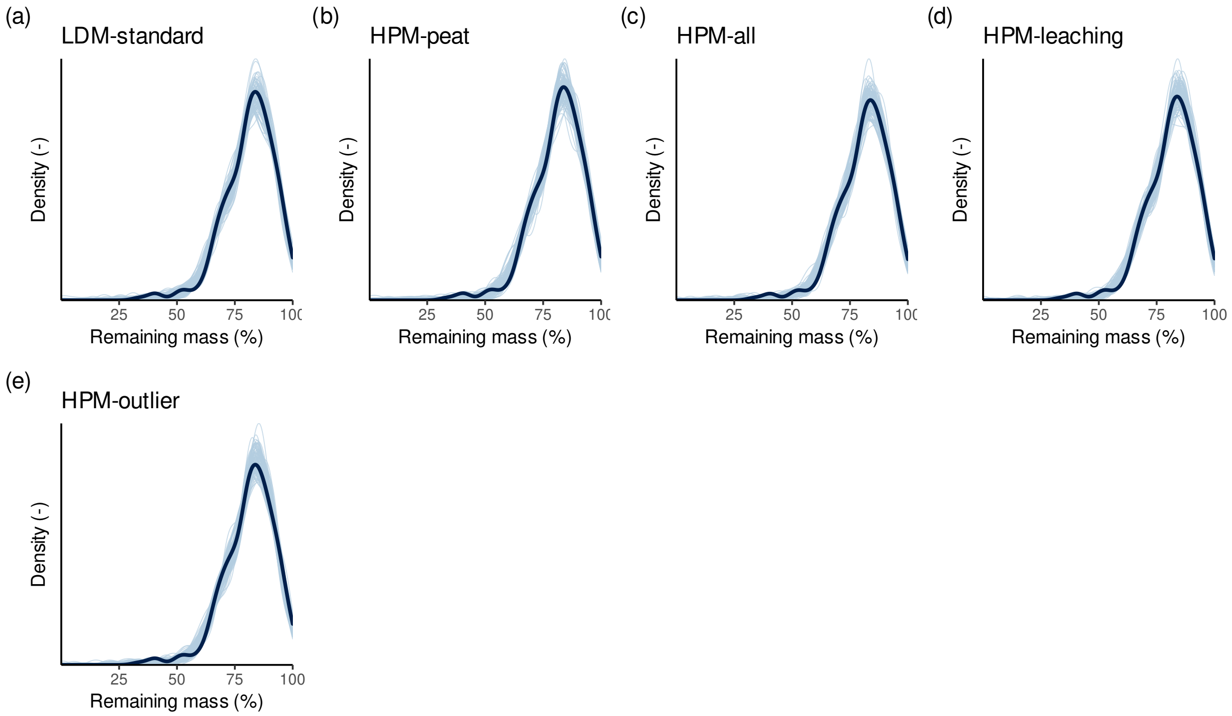


Figure S2: Density estimate of 100 sets of remaining masses sampled from the posterior distribution of each model (light blue lines) versus density estimate of the measured remaining masses from the litterbag studies.

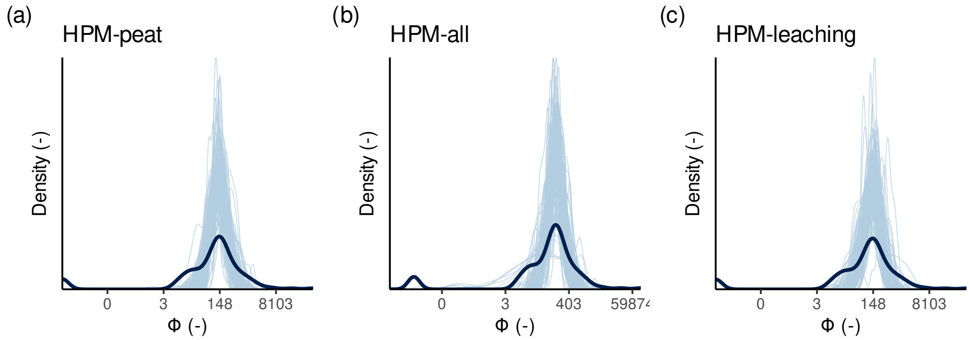


Figure S3: Density estimate of 100 sets of remaining mass errors (converted to precision) sampled from the prior distribution of each model (light blue lines) versus density estimate of the measured remaining mass errors from the litterbag studies. The x axis is log scaled.

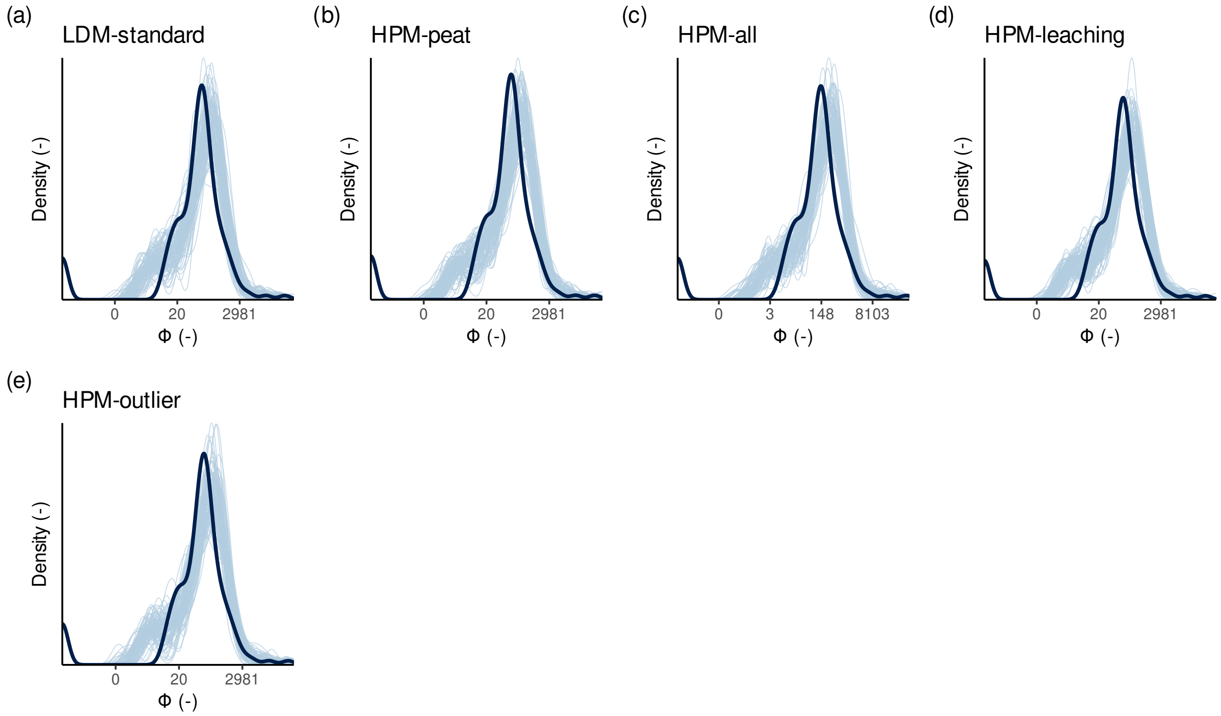


Figure S4: Density estimate of 100 sets of remaining mass errors (converted to precision) sampled from the posterior distribution of each model (light blue lines) versus density estimate of the measured remaining mass errors from the litterbag studies. The x axis is log scaled.

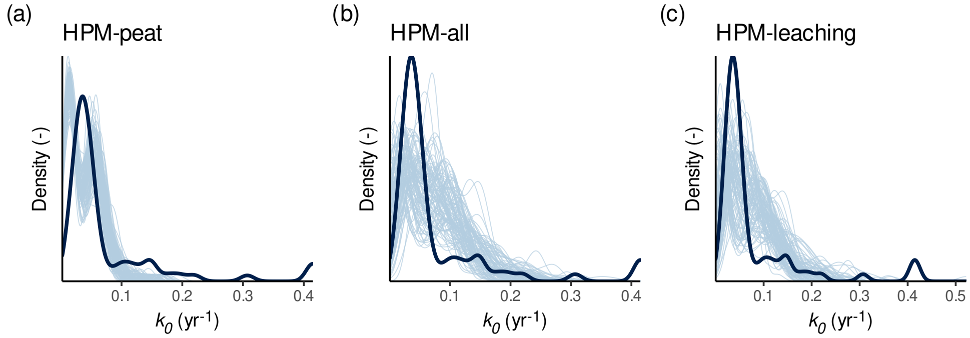


Figure S5: Density estimate of 100 sets of decomposition rates (k_0) predicted by the HPM modifications sampled from the prior distribution of each model (light blue lines) versus density estimate of the decomposition rates estimated from the litterbag studies.

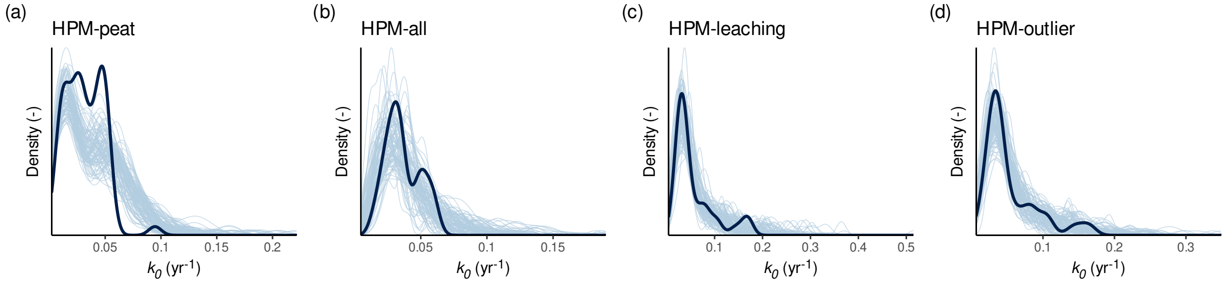


Figure S6: Density estimate of 100 sets of decomposition rates (k_0) predicted by the HPM modifications sampled from the posterior distribution of each model (light blue lines) versus density estimate of the decomposition rates estimated from the litterbag studies.

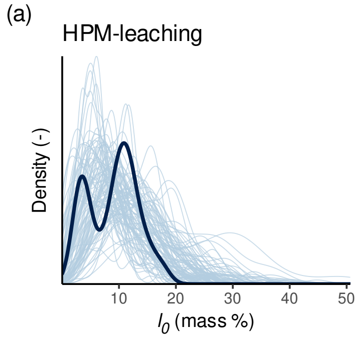


Figure S7: Density estimate of 100 sets of initial leaching losses (l_0) predicted by HPM-leaching sampled from the prior distribution (light blue lines) versus density estimate of the initial leaching loss estimated from the litterbag studies.

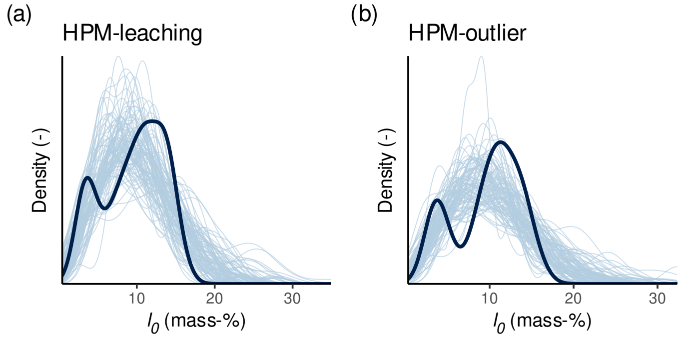


Figure S8: Density estimate of 100 sets of initial leaching losses (l_0) predicted by HPM-leaching sampled from the posterior distribution (light blue lines) versus density estimate of the initial leaching loss estimated from the litterbag studies.

S4 $k_{0,i}$ estimates in HPM-all and in HPM-leaching

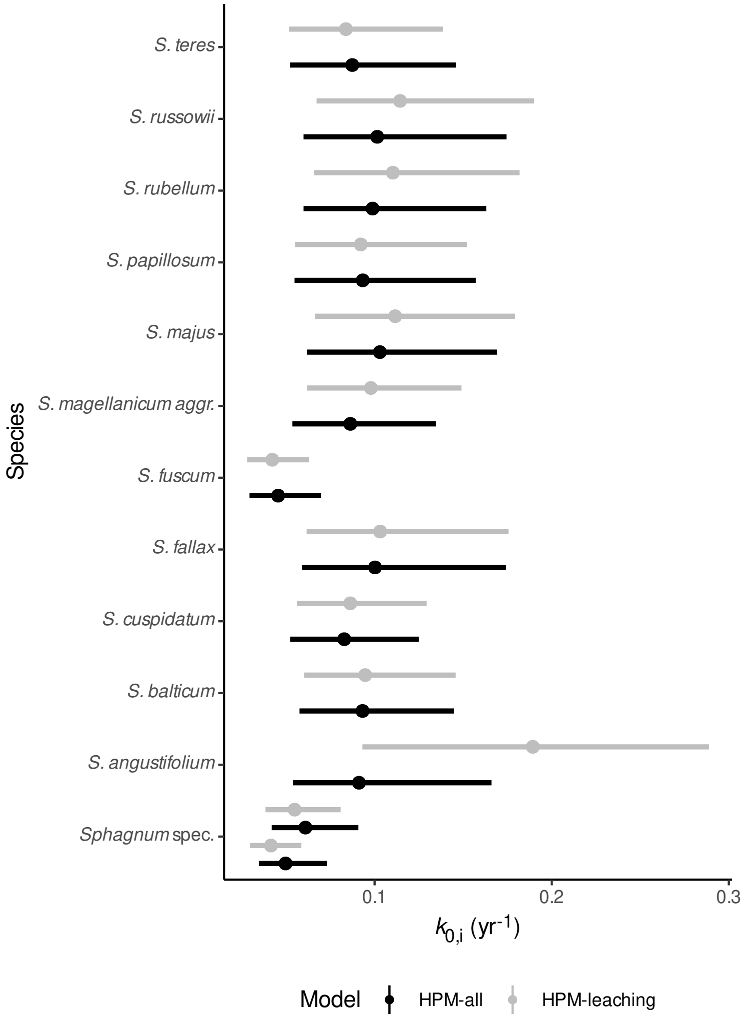


Figure S9: $k_{0,i}$ estimates in HPM-all and in HPM-leaching for each *Sphagnum* species. Points are average values and error bars are 95% confidence intervals. *Sphagnum* spec. are samples which have been identified only to the genus level and there are two values here because we defined two separate species in the HPM to estimate maximum possible decomposition rates separately for initial peat samples collected from 10 or 20 cm depth in Prevost et al. (1997).

S5 Marginal posterior distributions of HPM parameters in HPM-all and HPM-leaching

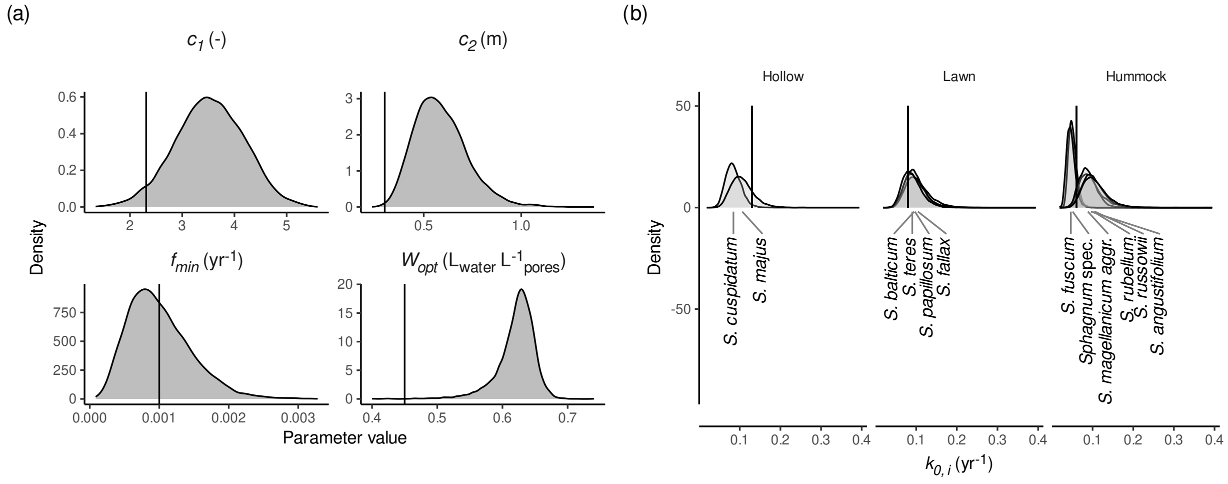


Figure S10: Marginal posterior distributions of HPM decomposition module parameters as estimated by HPM-all. (a) Marginal posterior distributions for c_1, W_{opt}, f_{min}, and c_2 (see Tab. 1 in the main text for details). Vertical black lines are the standard parameter values from Frolking et al. (2010). (b) Marginal posterior distributions for k_0 estimated for each species. Species were assigned to HPM microhabitats as described in the Methods section in the main text. *Sphagnum* spec. are samples which have been identified only to the genus level.

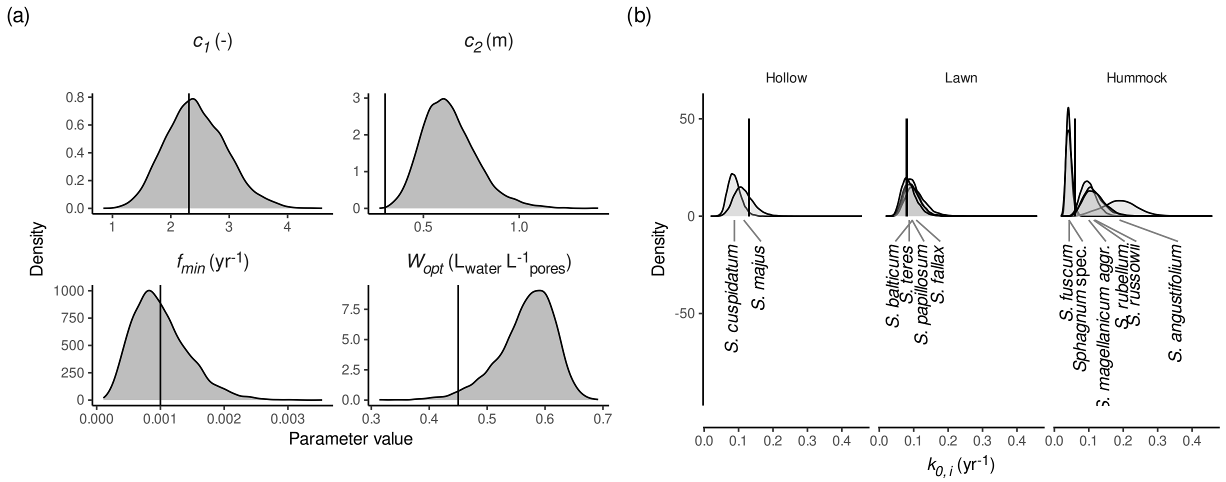


Figure S11: Marginal posterior distributions of HPM decomposition module parameters as estimated by HPM-leaching. (a) Marginal posterior distributions for c_1, W_{opt}, f_{min}, and c_2 (see Tab. 1 in the main text for details). Vertical black lines are the standard parameter values from Frolking et al. (2010). (b) Marginal posterior distributions for k_0 estimated for each species. Species were assigned to HPM microhabitats as described in the Methods section in the main text. *Sphagnum* spec. are samples which have been identified only to the genus level.

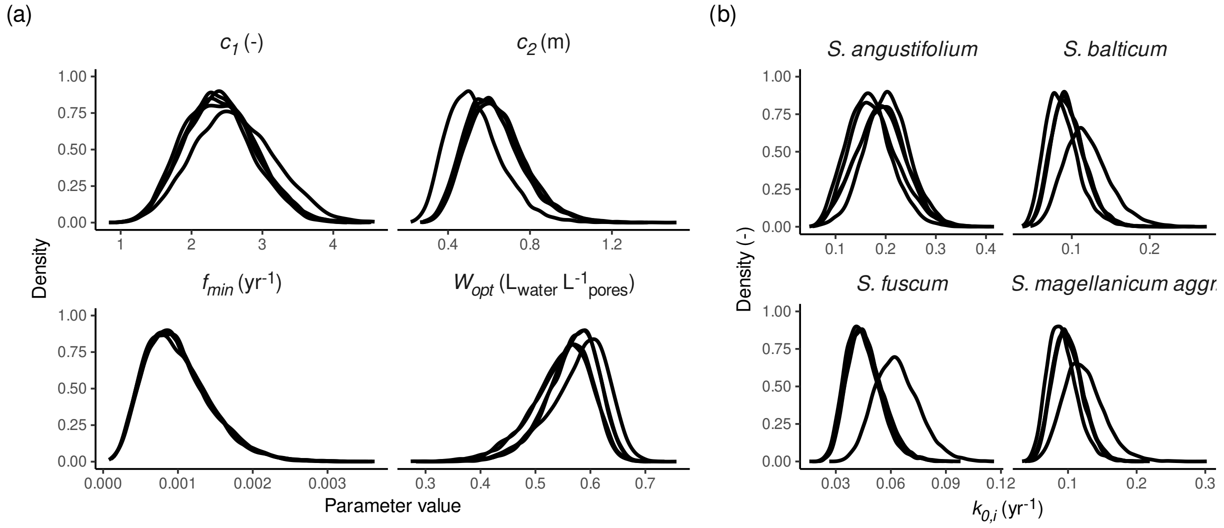


Figure S12: Marginal posterior distributions of HPM decomposition module parameters as estimated by HPM-leaching during the cross-validation. During the cross-validation, one of the cross-validation folds was left out each time and the model was refitted, producing a marginal posterior distribution for each parameter and cross-validation block. (a) Marginal posterior distributions for c_1, W_{opt}, f_{min}, and c_2 (see Tab. 1 in the main text for details). (b) Marginal posterior distributions for k_0 estimated for each species for which data were removed during the cross-validation.

S6 k_0 predicted by the HPM versus water table depth below the litter for different studies and species

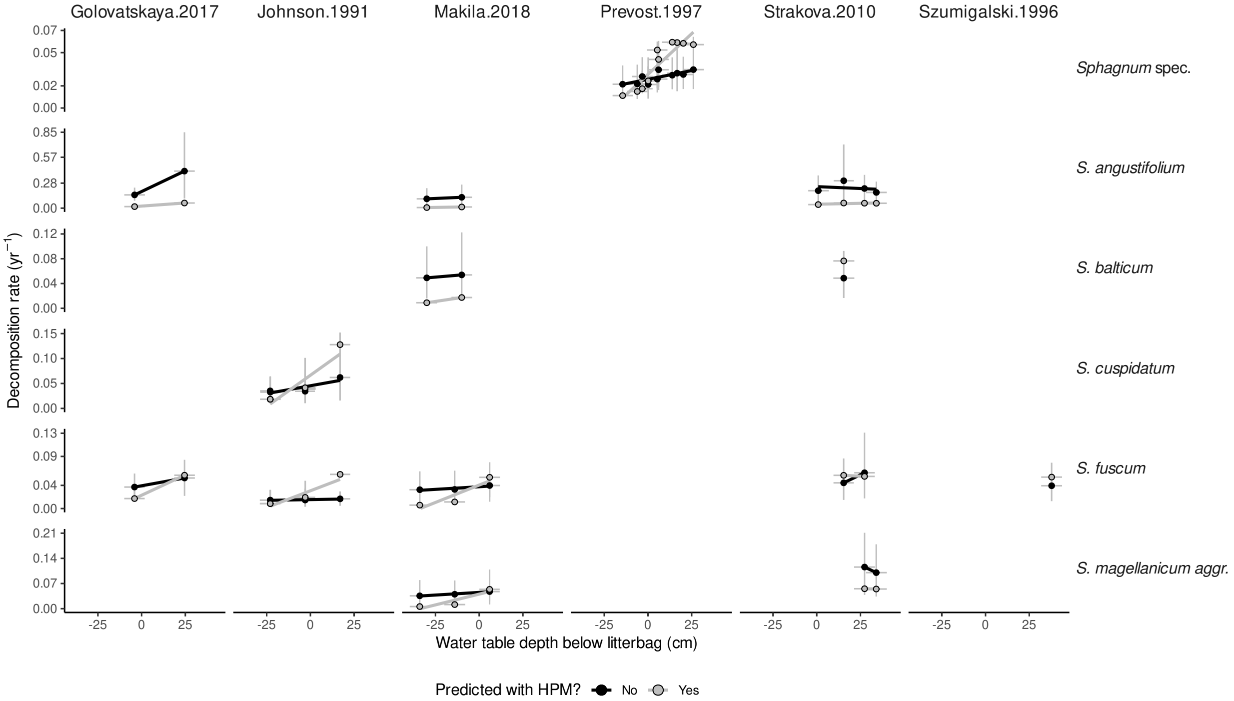


Figure S13: k_0 estimated with LDM-standard (Predicted with HPM = No) and predicted by the HPM decomposition module with standard parameter values (HPM-standard, Predicted with HPM = Yes) versus reported average water table depths below the litterbags for different species and studies (negative values represent litterbags placed below the water table, positive values represent litterbags placed above the water table in the unsaturated zone). Points represent average estimates and error bars 95% posterior intervals. Lines are predictions of linear models fitted to the average estimates. *Sphagnum* spec. are samples which have been identified only to the genus level. Only data for species with at least three replicates are shown. Error bars exceeding 0.5 yr^{-1} are clipped.

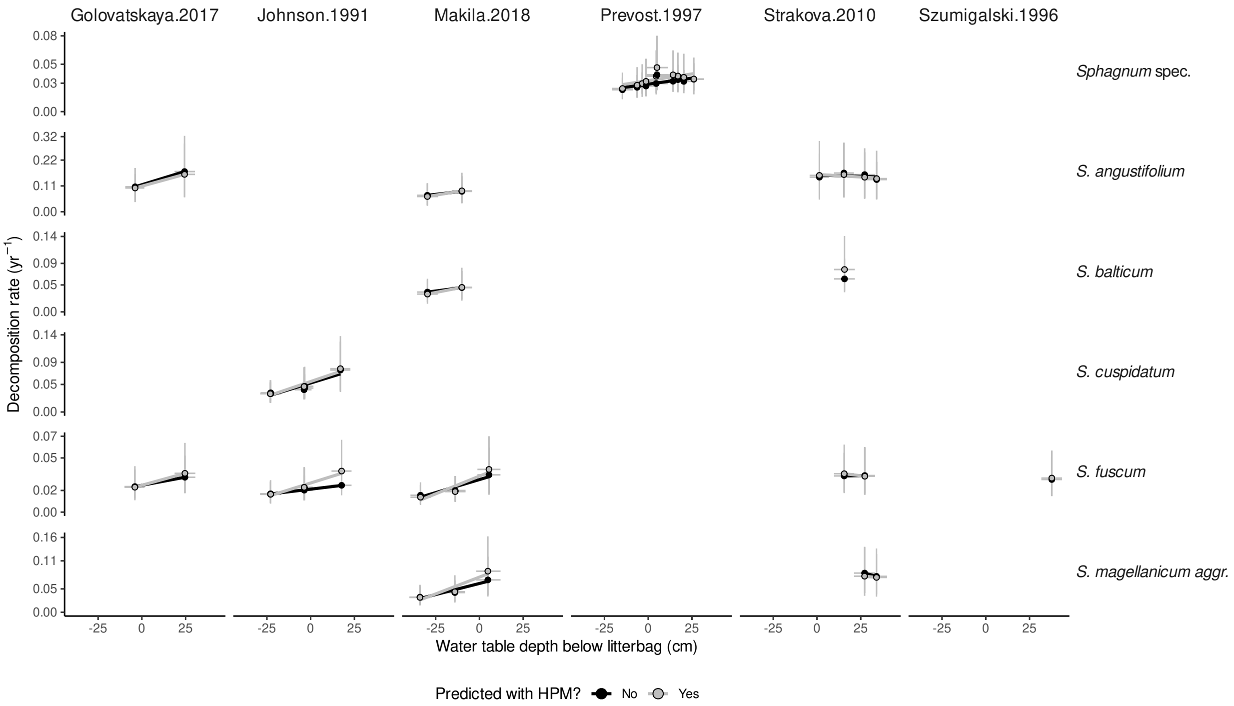


Figure S14: k_0 estimated with the litterbag decomposition model in HPM-leaching from the litterbag data (Predicted with HPM = No) and predicted by the HPM decomposition module with parameter values estimated from the litterbag data (HPM-leaching, Predicted with HPM = Yes) versus estimated average water table depths below the litterbags for different species and studies (negative values represent litterbags placed below the water table, positive values represent litterbags placed above the water table in the unsaturated zone). Points represent average estimates and error bars 95% posterior intervals. Lines are predictions of linear models fitted to the average estimates. *Sphagnum* spec. are samples which have been identified only to the genus level. Only data for species with at least three replicates are shown. Error bars exceeding 0.5 yr^{-1} are clipped.

S7 Depth profiles of predicted decomposition rates with W_{opt} estimated by HPM-leaching or set to its standard value for *S. fallax*

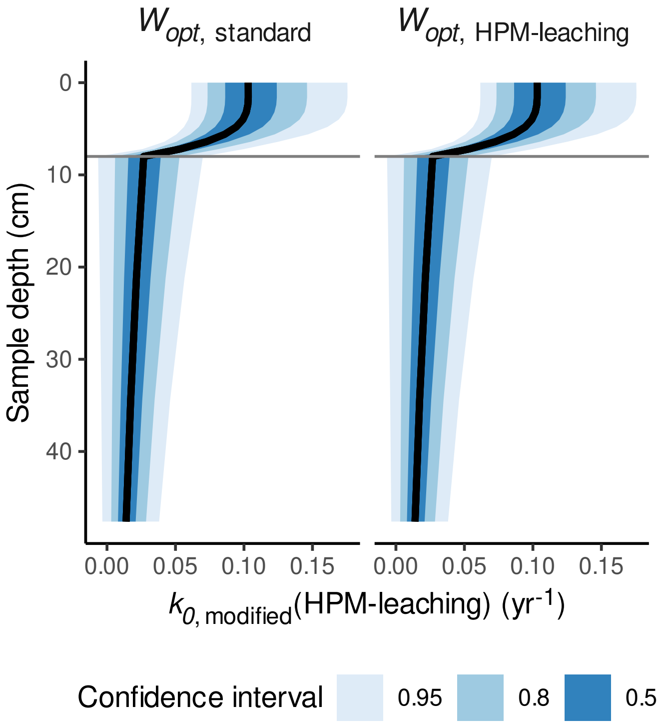


Figure S15: Decomposition rates predicted with HPM-leaching ($k_{0,\text{modified}}$(HPM-leaching)) for *S. fallax* (hollows), using either the standard value for W_{opt} or the W_{opt} value estimated by HPM-leaching versus depth of the litter below the peat surface. The horizontal line is the average water table depth.

S8 Results for HPM-outlier

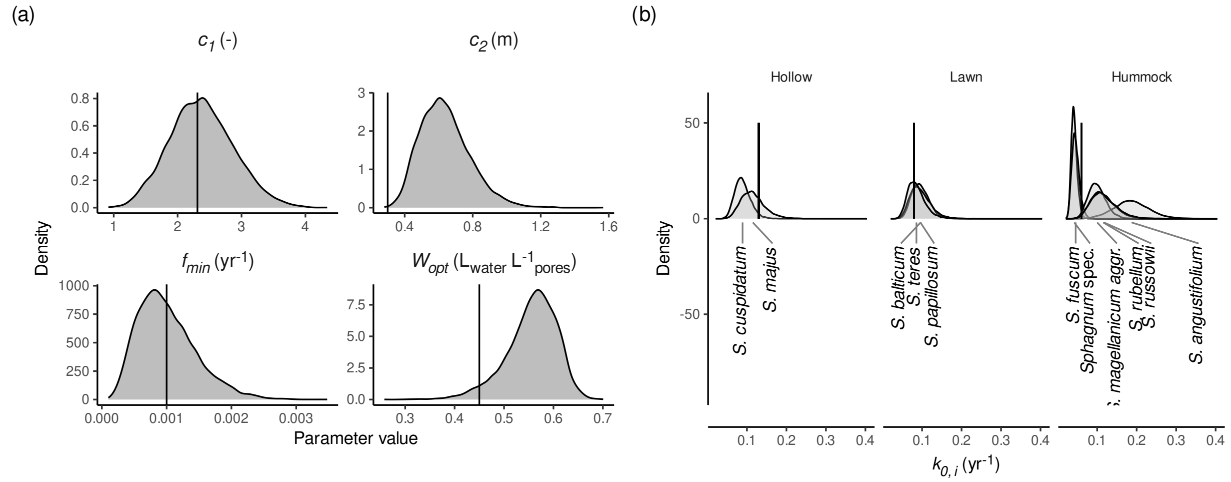


Figure S16: Marginal posterior distributions of HPM decomposition module parameters as estimated by HPM-outlier. (a) k_0 estimated for each species. Species were assigned to HPM microhabitats as described in the Methods section in the main text. (b) other HPM parameters. Vertical black lines are the standard parameter values from Frolking et al. (2010). *Sphagnum* spec. are samples which have been identified only to the genus level.

S9 Prediction uncertainties of HPM-leaching

To illustrate that the HPM decomposition module implies large uncertainties if its parameters are estimated from available litterbag data, we simulate decomposition of *S. fallax* and *S. fuscum* litter during 50 years, either incubated at 10 cm depth under a degree of saturation of 0.6 $\mathrm{L_{water}\ L_{pores}^{-1}}$, or 20 cm below the water table. The results are shown in Fig. S17.

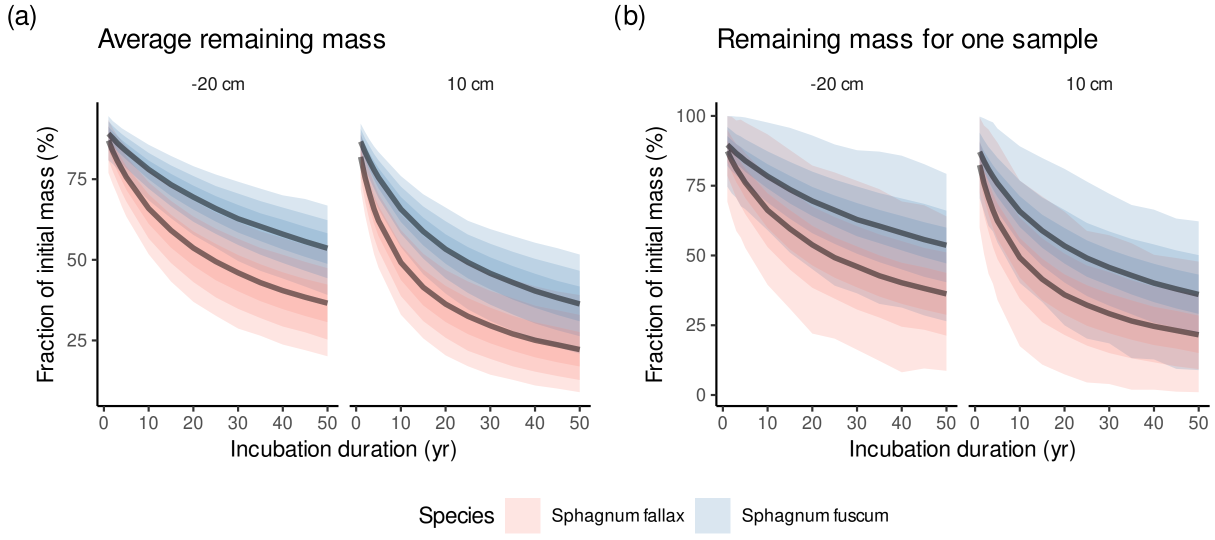


Figure S17: Fraction of initial mass remaining of *S. fuscum* and *S. fallax* versus incubation duration as predicted by HPM-leaching, assuming average species α and uncertainty of remaining masses averaged across litterbag experiments. (a) Shows predicted fractions of initial mass remaining and (b) predicted fractions of initial mass remaining for one individual sample. Samples are either incubated in the saturated zone 20 cm below the water table, or in the unsaturated zone 10 cm above the water table. Shaded areas are 50, 80, and 95% confidence and prediction intervals, respectively.

S10 R code to predict k_0, l_0, and remaining masses with HPM-leaching

HPM-leaching and functions to predict k_0 and l_0 for different species and water table levels are available via the R package hpmdpredict (Teickner and Knorr, 2025). To make predictions, one first has to define some variables like the incubation duration. Here, we predict remaining masses and initial leaching losses for *S. fuscum* incubated at a degree of saturation of 0.6 $\mathrm{L_{water}\ L_{pores}^{-1}}$ during the first five years.

```
d <-
  tibble::tibble(
    incubation_duration = seq(from = 0, to = 5, length.out = 30),
    m0 = 1,
    layer_degree_of_saturation_1 = 0.6,
    layer_water_table_depth_to_surface_1 = 20,
    sample_depth_lower = 10,
    hpm_taxon_rank_value = "Sphagnum fuscum"
  )
```

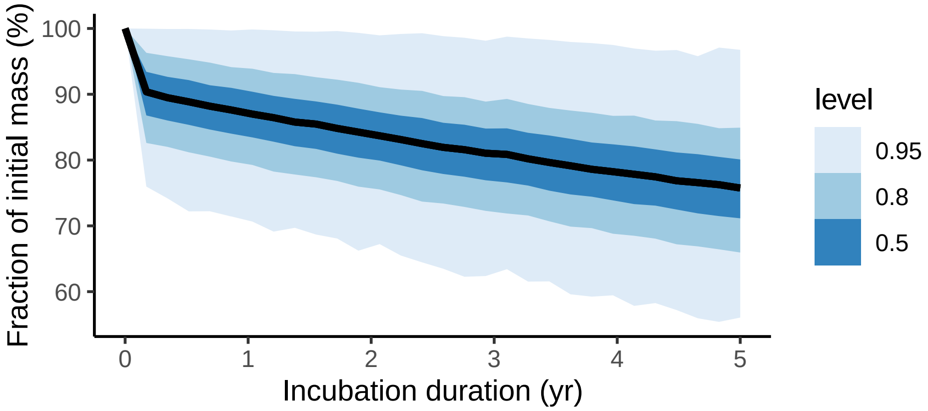
Next, one can pass this data frame to `hpmd_predict_fit_4()` which makes the predictions.

```
library(hpmdpredict)
d <- hpmdpredict::hpmd_predict_fit_4(newdata = d)
```

To illustrate the result, we plot predicted remaining masses versus incubation time:

```
library(ggplot2)
library(ggdist)

d |>
  ggplot(aes(ydist = mass_relative_mass * 100, x = incubation_duration)) +
  stat_lineribbon() +
  scale_fill_brewer() +
  labs(
    y = "Fraction of initial mass (%)",
    x = "Incubation duration (yr)"
  )
```



Further information are available from the package documentation.

References

Bürkner, P.-C., Gabry, J., Kay, M., and Vehtari, A.: posterior: Tools for working with posterior distributions, 2023.

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.

Gabry, J. and Mahr, T.: bayesplot: Plotting for bayesian models, 2022.

Kallioinen, N., Paananen, T., Bürkner, P.-C., and Vehtari, A.: Detecting and diagnosing prior and likelihood sensitivity with power-scaling, Statistics and Computing, 34, 57, https://doi.org/10.1007/s11222-023-10366-5, 2024.

Kay, M.: ggdist: Visualizations of distributions and uncertainty, Manual, https://doi.org/10.5281/zenodo.3879620, 2022a.

Kay, M.: tidybayes: Tidy data and geoms for Bayesian models, https://doi.org/10.5281/zeno do.1308151, 2022b.

Liu, H. and Lennartz, B.: Hydraulic properties of peat soils along a bulk density gradient-A meta study, Hydrological Processes, 33, 101–114, https://doi.org/10.1002/hyp.13314, 2019.

Pedersen, T. L.: patchwork: The composer of plots, 2020.

Prevost, M., Belleau, P., and Plamondon, A. P.: Substrate conditions in a treed peatland: Responses to drainage, Écoscience, 4, 543–554, https://doi.org/10.1080/11956860.1997.11682434, 1997.

R Core Team: R: A language and environment for statistical computing, Manual, R Foundation for Statistical Computing, Vienna, Austria, 2022.

Teickner, H. and Knorr, K.-H.: hpmdpredict: Predictions with model HPM-leaching from Teickner et al. (2024), https://doi.org/10.5281/ZENODO.14724314, 2025.

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, 2025.

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

Wickham, H.: ggplot2: Elegant graphics for data analysis, 2nd ed. 2016., Springer International Publishing : Imprint: Springer, Cham, https://doi.org/10.1007/978-3-319-24277-4, 2016.

Wickham, H., Averick, M., Bryan, J., Chang, W., McGowan, L., François, R., Grolemund, G., Hayes, A., Henry, L., Hester, J., Kuhn, M., Pedersen, T., Miller, E., Bache, S., Müller, K., Ooms, J., Robinson, D., Seidel, D., Spinu, V., Takahashi, K., Vaughan, D., Wilke, C., Woo, K., and Yutani, H.: Welcome to the Tidyverse, Journal of Open Source Software, 4, 1686, https://doi.org/10.21105/joss.01686, 2019.