



Supplement of

**Assessing forest biomass and productivity with data-driven
vegetation indices: insights from 900 000 simulated forest stands**

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S1 Updates and parameterization of the radiative transfer model mSCOPE

In this supplement, we describe how we adjusted and parameterized the radiative transfer model mSCOPE to couple it with the forest model FORMIND.

S1.1 Support of vertically heterogeneous leaf densities

- 5 FORMIND models the vertical leaf distribution in forest patches explicitly (Henniger et al., 2023a). This contrasts with the classical mSCOPE, which builds on the assumption of a vertically homogeneous leaf density (Verhoef, 1998). Hence, some adjustments were necessary to accurately incorporate the heterogeneous leaf densities resulting from FORMIND into mSCOPE simulations:
- The discretization scheme needed to be adjusted.
- 10 – The probability P_{so} that a leaf is both directly lit by the sun and directly visible to the observer needed to be computed differently to accurately account for hot-spot effects.

Below we first explain corresponding adjustments to the general model setup; then we show how we discretized the vertical leaf distribution; finally, we discuss necessary model adjustments to capture hot-spot effects.

S1.1.1 General setup

- 15 The mSCOPE model can be formulated as a four-stream ODE system (Yang et al., 2017)

$$\frac{1}{L} \frac{dE_s}{dx} = kE_s \tag{S1}$$

$$\frac{1}{L} \frac{dE^-}{dx} = -sE_s + aE^- - \sigma E^+ \tag{S2}$$

$$\frac{1}{L} \frac{dE^+}{dx} = s'E_s + \sigma E^- - aE^+ \tag{S3}$$

$$\frac{1}{L} \frac{dE_o}{dx} = wE_s + vE^- + v'E^+ - KE_o, \tag{S4}$$

- 20 where E_s is the direct solar flux, E^- the diffuse downward flux, E^+ the diffuse upward flux, and E_o the flux in viewing direction; k , K , s , s' , a , σ , v , v' , and w are coefficients dependent on the height x ; and L is the (constant) leaf density. We may write the system (S1)-(S4) in vector notation as

$$\frac{1}{L} \frac{dE}{dx} = f(E), \tag{S5}$$

- 25 where E denotes the vector of the four fluxes and f is a vector-valued function modelling how the fluxes change in interactions with leaves.

By making the coefficients dependent on height, the model accounts for vertically heterogeneous leaf properties. The leaf density, however, is assumed to be constant throughout the canopy. This made it possible to express the integration over the leaf distribution as an integration over space, as in (S1)-(S4) and (S5):

$$\frac{dE}{dl} = \frac{dx}{dl} \frac{dE}{dx} = \frac{1}{L} \frac{dE}{dx}, \tag{S6}$$

- 30 where $l(x) = Lx$ is the number of leaf layers below height x . If the leaf density changes with height x , we need to consider the density gradient $\frac{dx}{dl}$. This may be approximated as $\frac{\Delta x(j)}{\Delta l(j)}$, where $\Delta x(j)$ is the height of leaf layer j and $\Delta l(j)$ the corresponding leaf area index (LAI). Hence, the discretized version of (S5) can be formulated as follows:

$$E(j+1) = E(j) + f(E(j))\Delta l(j). \tag{S7}$$

That is, the integration scheme of the mSCOPE model still applies, though Δl needs to be adjusted in each height layer.

35 S1.1.2 Discretization of the forest canopy

To solve system (S1)-(S4), Yang et al. (2017) discretize the canopy into 60 thin leaf layers. They note that the leaf layers must be thin enough so that the LAI per height layer does not exceed approximately 0.1 so as to guarantee numerical stability. In this paper, we used the height discretization of the forest model FORMIND, which splits the forest into vertical layers of 0.5 m height. However, with this approach, LAI values per layer exceeding 0.1 are possible. Hence, we split each FORMIND layer j with $\Delta l(j) > 0.1$ into $\lceil \Delta l(j)/0.1 \rceil$ sublayers prior to applying mSCOPE. Furthermore, we excluded all empty layers, as they do not affect the computed reflectance values and cause numerical issues. As a result, the number of layers depended on the structure of the considered forest.

S1.1.3 Hot spot effects

In mSCOPE, the light reaching the observer is computed as a weighted sum of the individual fluxes reaching the observer from each individual height layer:

$$E_o(j_{\max}) = \sum_{j=1}^{j_{\max}} w(j) E_s P_{so}(j) + (v(j) E^-(j) + v'(j) E^+(j)) P_o(j).$$

Here, $P_o(j)$ is the probability that a light ray emitted at layer j escapes the forest, and $P_{so}(j)$ is the bi-directional gap probability, i.e., the probability that a light beam from the sun reaches layer j and escapes the forest. Incorporating P_{so} explicitly is necessary to account for hotspot effects, occurring when the sun and the view direction coincide, so that all visible leaves are directly lit by sunlight. While most of the dynamics of the mSCOPE model such as light transmission, scattering and reflection are driven by the leaf density and not directly dependent on the forest height, the probability P_{so} decreases as individual leaf layers are farther apart from one another, making leaf positions less correlated (Verhoef, 1998). Hence, in forests with equal LAI, the hot spot effects will be stronger the denser the leaf layers are packed.

Yang et al. (2017) compute P_{so} following the work of Verhoef (1998, pp. 153ff). He computes the probability $P_{so}(j)$ based on probabilities $p_{so}(i, j)$, denoting the likelihood that a light ray reflected in layer j passes through a layer i both from the sun direction and in observer direction. If the two directions are significantly different and the layers i and j are far apart from each other, the horizontal position where the rays in downward and upward direction pass layer j will be far apart from one another. As a consequence, the events of the rays passing through the layer in either direction are almost uncorrelated and independent of layer i where the beam was reflected, i.e., where the rays from the sun and to the observer intersect:

$$60 \quad p_{so}(i, j) \approx p_s(j) p_o(j). \quad (\text{S8})$$

Here, $p_s(j)$ is the probability that a ray from the sun passes layer j , and $p_o(j)$ is the probability that a ray to the observer passes the layer. In contrast, if the two directions coincide or the reflection point is close to the considered layer j , the horizontal locations where layer j is passed in each direction are close together, and the “passing events” are correlated.

Verhoef (1998) calls the correlation coefficient between the two events $\rho(i, j)$ and models it as exponentially decaying with (1) the distance $d(i, j)$ at which the two rays pass layer j multiplied by (2) the inverse of a correlation length constant ℓ , dependent on the leaf size, shape, and inclination:

$$\rho(i, j) = \exp\left(-\frac{d(i, j)}{\ell}\right), \quad (\text{S9})$$

where

$$d(i, j) = (x(j) - x(i)) \sqrt{\tan^2 \theta_s + \tan^2 \theta_o - 2 \tan \theta_s \tan \theta_o \cos \psi}, \quad (\text{S10})$$

70 is computed based on geometrical considerations (c.f. Fig. 8.1 in Verhoef, 1998) with $x(j)$ being the height of layer j above the ground. As computing ℓ from other parameters is complex, Verhoef (1998) assumes it is a given constant. Using the definition

of the correlation coefficient, he obtains

$$p_{so}(i, j) = p_s(j)p_o(j) + \rho(i, j)\sqrt{p_s(j)p_o(j)(1 - p_s(j))(1 - p_o(j))} \quad (\text{S11})$$

$$= p_s(j)p_o(j) + \exp\left(-\frac{d(i, j)}{\ell}\right)\sqrt{p_s(j)p_o(j)(1 - p_s(j))(1 - p_o(j))}. \quad (\text{S12})$$

- 75 If the leaf density is constant, $p_s(j)$ and $p_o(j)$ are independent of the layer j , and both p_{so} and P_{so} can be derived in closed form via integrals over continuous space (Verhoef, 1998, pp. 154f) or, equivalently, the cumulative leaf density. If the leaf density is different in each layer, however, we may fall back to the discrete model version and compute the probability P_{so} as

$$P_{so}(j) = \prod_{k=j}^{j_{\max}} p_{so}(i, k).$$

- As $P_{so}(j)$ needs to be computed for each layer, this algorithm runs in $\mathcal{O}(n^2)$, where n is the number of considered layers.
80 This can be inefficient. However, if the correlation $\rho(i, k)$ is small for $k > j_0$ for some j_0 , it is $p_{so}(i, k) \approx p_s(k)p_o(k)$, and we can write

$$P_{so}(j) \approx \left(\prod_{k=j}^{j_0} p_{so}(i, k) \right) \left(\prod_{k=j_0+1}^{j_{\max}} p_s(k)p_o(k) \right). \quad (\text{S13})$$

$$= P_s(j_0 + 1)P_o(j_0 + 1) \prod_{k=j}^{j_0} p_{so}(i, k), \quad (\text{S14})$$

- where $P_s(j_0 + 1)$ is the probability that a light ray from the sun reaches layer $j_0 + 1$ undisturbed, and $P_o(j_0 + 1)$ is the
85 probability that a light ray from layer $j_0 + 1$ reaches the observer undisturbed. Equation (S14) can be computed for all layers in $\mathcal{O}(n)$, since the number $j_0 - j$ of layers with a significant correlation is bounded by a constant. We defined j_0 as the first layer j where $\rho(i, j) < 10^{-5}$.

Following Yang et al. (2017), we computed the correlation length ℓ as

$$\ell = \frac{2w_l}{k + K}, \quad (\text{S15})$$

- 90 where w_l is the (species-dependent) width of a leaf, which we assumed to be 5 cm independent of the height of the considered layer.

S1.2 Reduced sunfleck observation on soil

- The probability $P_{so}(0)$ that a location on the ground is both directly lit by sunlight (sunfleck) and visible to the observer is generally computed according to Eq. (S14). Depending on the parameterization and the forest density, sunflecks can account for
95 a major share of the computed reflectance, especially for short wavelengths. However, the structure and cover of the ground (grass / herb cover, deadwood, etc.) are typically unknown and may significantly reduce the visible ground portion. To account for this issue and reduce the potential for bias, we set $P_{so}(0) = 0$ in this study. This model adjustment does not invalidate the modelled energy fluxes, as reflection of light into the diffuse upward stream is still considered. Instead, we made the additional assumption that no sunlit ground is directly visible to the observer.

100 S1.3 Parameterization of the radiative transfer model

We based our parameterization of mSCOPE on the work of Henniger et al. (2023a) but adjusted the leaf parameters based on values from the TRY data base (Kattge et al., 2011) where available. We submitted a TRY data request on July 30th 2024 regarding data on the leaf chlorophyll content per leaf area and the leaf carotenoid content per leaf area. We refined the resulting

	Pinus	Picea	Fagus	Quercus	Populus	Betula	Robinia
Chlorophyll a+b content $\left[\frac{\mu\text{g}}{\text{cm}^2} \right]$	56	37	41	31	44	29	36.71
Leaf mass per unit area $\left[\frac{\text{g}}{\text{cm}^2} \right]$	0.024	0.025	0.014	0.014	0.007	0.006	0.006
Equivalent water thickness [cm]	0.003	0.003	0.017	0.017	0.009	0.0102	0.0102
Senescence material (brown pigments) [–]	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Carotenoid content $\left[\frac{\mu\text{g}}{\text{cm}^2} \right]$	12.5	7.5	10	8	9.38	6.9	8.62
Leaf structure parameter [–]	1.25	1.24	2.6	2.6	1.30	1.77	1.77

Table S1. Adjusted parameters for the considered genera.

data to include only species of the considered genera and filtered the data by the respectively most frequent unit, namely g/m^2 for the chlorophyll content and $\mu\text{g}/\text{cm}^2$ for the carotenoid content. The selected data were originally published by Medlyn et al. (1999) and Lukeš et al. (2013) for the chlorophyll content and Lukeš et al. (2013) for the carotenoid content.

We computed the mean of the chlorophyll and carotenoid content for each genus. No chlorophyll content estimates were available for Populus, so we kept the original value used in Henniger et al. (2023a). For the carotenoid content, estimates were only available for Pinus, Picea, and Betula. We kept the other values by Henniger et al. (2023a) but noted that the updated carotenoid values for Pinus and Picea were significantly higher than the originals. Furthermore, we noted that the updated carotenoid / chlorophyll ratio of all genera except Fagus and Quercus was about 1/4. Hence, we adjusted the carotenoid content for these genera based on the latter carotenoid / chlorophyll ratio to avoid issues arising from inconsistent data adjustment. The resulting optical leaf parameters we used are displayed in Table S1.

S2 Description of the Monte Carlo approach to generate forest stands (“Forest Factory”)

S2.1 Background and previous work

In this paper, we generated forest stands via a Markov Chain Monte Carlo (MCMC) approach. Our method is based on the “Forest Factory”, introduced by Bohn and Huth (2017) and further improved by Henniger et al. (2023b). The goal of the Forest Factory is to construct large numbers of forest stands with different structure and species composition by randomly adding trees to a forest as long as it is in an ecologically feasible state. A stand is considered feasible if the GPP of each tree suffices to satisfy its respiratory needs. Hence, the state space of possible forests consists of all those stands where each tree is sufficiently productive. The state space can be filtered by further constraints, such as available space.

The original idea of the Forest Factory was to conduct a hierarchical sampling approach to randomly generate possible forest states: first, a minimal and a maximal tree height $h_{\min}$, $h_{\max}$ is drawn from some stochastic distribution; second, a set of species that can attain heights in $[h_{\min}, h_{\max}]$ is randomly assembled; and third, a maximal crown volume V is randomly drawn. Then, the forest stand is filled with trees by first drawing tree heights in $[h_{\min}, h_{\max}]$ and then corresponding species from the species pool until the forest stand is “full”, i.e., the crown volume V has been reached or another constraint is not fulfilled (space or productivity constraint).

If only the productivity constraint is violated, i.e., despite enough space in the forest, there are trees whose maintenance respiration exceeds their GPP, an attempt is made to bring the forest stand into a feasible state by changing the species of the trees in question. If trees with insufficient GPP can be replaced by trees with different species but the same heights, more trees are added to the forest until no addition is possible. That way, the chances of reaching the target crown volume V increase. In summary, the Forest Factory attempts to generate forests that match the pre-sampled forest characteristics as well as possible.

In this study, we took a slightly different approach motivated by the following considerations. First, the original approach can yield forest states in which some trees are not able to fulfill their respiratory needs. This is because any species adjustment made to satisfy the productivity constraint also affects the productivity of other trees, potentially making them violate the productivity constraint, in turn. In favour of computational efficiency, Henniger et al. (2023b) did not consider such secondary effects in already processed trees, potentially leading to infeasible states. Second, every adjustment to the forest state would require updating the productivity of all trees considering water and light competition, which, in turn, is computationally costly. Therefore, the original Forest Factory took a simplified approach not taking the entire year’s climate into account when updating the productivity of trees. Third, the optimization approach attempting to find more suitable species for trees whose GPP fell below their maintenance respiration leads to a bias towards species with higher carbon use efficiency. Fourth, the approach makes it difficult to interpret the results in a statistically rigorous manner.

S2.2 Revised algorithm of the Forest Factory

We updated the Forest Factory approach by dropping the step of pre-sampling the crown volume (first drawing a “target crown volume”, then assembling a forest with this crown volume) and considering the crown volume as an emerging property, i.e., sampling from forest states with the given height range and species pool. Similar to Henniger et al. (2023b), we started by drawing a height range, a species pool, and a year-long climate sequence. Then we added and removed trees randomly, so that the forest emerging after many addition / removal steps could attain both small and large crown volumes. As we did not attempt to reach a specific target crown volume, no optimization step adjusting tree species was necessary. Instead, we accepted all steps where none of the constraints was violated and rejected all other steps, falling back to the respective previous state. After a limited number of iterations, we terminated the process. Below we provide further details.

S2.2.1 Feasibility

We sought to simulate forests that satisfy the following constraints: (1) the GPP of each tree should be at least as high as its required maintenance respiration (“productivity constraint”), and (2) the forest’s crown area should not exceed the forest area in any height level (“space requirement constraint”). If a forest state satisfies all criteria, we call it “feasible”.

To evaluate whether a forest stand was feasible, we first checked the space constraint, as it is easy to verify based on the crown dimensions of the trees and does not require simulation of carbon fluxes. If the space constraint was satisfied, we computed the total GPP and maintenance respiration for all trees in the stand for one year, taking into account water and light competition as well as temperature effects. Then we checked for each tree whether its GPP satisfied its respiratory needs.

S2.2.2 Pre-sampling

Before generating a forest stand, we randomly drew a minimal and a maximal height $h_{\min}$, $h_{\max}$ uniformly from the interval $[5.8\text{m}, 50\text{m}]$. Then we determined the set $S_{h_{\min}}$ of species that can attain heights of at least $h_{\min}$. Next, we drew a number N from the discrete uniform distribution over the set $\{1, \dots, |S_{h_{\min}}|\}$, where $|\cdot|$ denotes the number of elements. Finally, we drew N species from $S_{h_{\min}}$ under the condition that at least one of the selected species can reach height $h_{\max}$. The resulting set $\tilde{S}$ contained the species pool for the next generated forest. These pre-sampling steps followed the approach by Henniger et al. (2023b). Lastly, we randomly drew a climate sequence with a daily resolution and a length of one year.

S2.2.3 Steps

Starting from an initial forest (see below), we iteratively changed the forest state by adding or removing trees. Let X_i denote the forest state after i attempts to change it. We generated the next forest state X_{i+1} as follows: with probability 0.5, we either randomly added or removed a tree to / from X_i (details below), arriving at a new forest state X'_i . Then we checked if the proposed state X'_i was feasible. If it was, we accepted the proposed state, setting $X_{i+1} := X'_i$, making it the new forest state. Otherwise, we rejected the change, $X_{i+1} := X_i$, leaving the forest state unchanged.

As the feasibility check is computationally costly, we used an adaptive step size k between consecutive feasibility checks. That is, we performed k tree additions or removals and rejected all changes jointly if the resulting proposed state was infeasible.

175 We started with a step size of $k = 5$ and adjusted the step size dynamically during the simulation based on the success of previous feasibility checks. When 5 consecutive feasibility checks were successful, we doubled k ; when 5 consecutive feasibility checks were unsuccessful, we divided it by 2 (rounding down to the next integer). However, we never allowed step sizes below 1 and refrained from further step size increases if $k \geq 10$.

S2.2.4 Initialization

180 To reduce the required burn-in time until the simulation reaches its limiting distribution, we did not start with an empty forest (“bare ground”) but from a “half-full” forest. To that end, we randomly added trees to the forest (see next section for details on how the trees’ properties were selected) until their crown occupied half of the volume that a forest of height of $h_{\max}$ could attain, i.e., $h_{\max} \cdot A$, where $A = 0.04$ ha is the ground surface area of the forest stand. Then we evaluated the feasibility of the forest stand. If the forest stand was infeasible, we randomly removed half of the trees and checked the feasibility again. If
185 the state was still not feasible we repeated this procedure until a feasible state was found. Note that an empty forest (no trees) always satisfies the feasibility constraints.

S2.2.5 Adding / removing a tree

When adding a tree, we randomly drew its height h from a conditional exponential distribution with rate parameter $\lambda = 0.05$, conditioned to the interval $[h_{\min}, h_{\max}]$ using the inversion method (Henniger et al., 2023b). Next, we determined the set
190 $S_h \subseteq S_{h_{\max}}$ of all species that could attain a height of h . Finally, we randomly drew the tree’s species from the set S_h . In FORMIND, tree height and species suffice to fully characterize a tree, and all other static properties (e.g. DBH, crown diameter, etc.) can be computed from this information via allometric relationships.

When removing a tree, we randomly selected any of the forest stand’s trees and removed it. In cases where the forest was empty and no trees could be removed, we switched to adding a tree instead.

195 S2.2.6 Termination

We terminated the procedure after a number of at least 200 individual tree additions and removals had been reached. In the hypothetical case that the final forest did not contain any tree, we continued attempting to add a tree until at least one tree was present. Note that only in exceptional cases with very harsh climatic conditions, forest states with a single tree could be infeasible.

200 S3 Distributions of key characteristics of the generated forests

In this study, we generated large numbers of 0.04 ha forest stands via a Markov-Chain-Monte-Carlo-type approach. These forests differed greatly in their species composition and heterogeneity. The distributions of key forest characteristics among the data set are displayed in Fig. S1. Besides the forest attributes used in this study, we also plotted the distribution of the basal-area-weighted Shannon entropy in the forest stands. In contrast to the classical Shannon entropy, this diversity measure
205 also incorporates the size (basal area) of the individuals rather than only their number. That is, the entropy is maximized, when all present species have the same basal area rather than the same abundance.

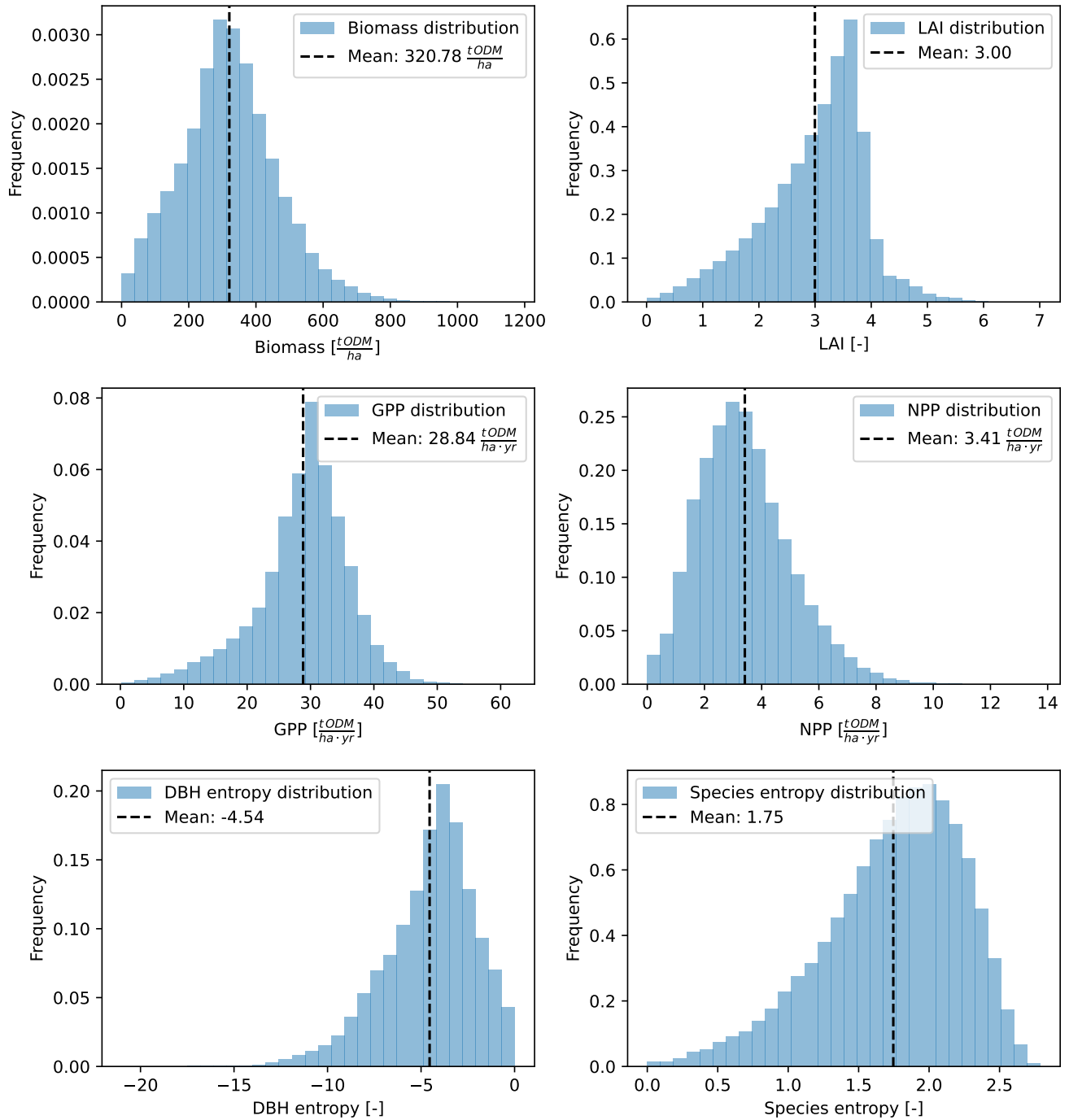


Figure S1. Distributions of the key forest characteristics considered in this study. DBH entropy refers to the basal-area weighted DBH entropy (Fischer et al., 2024). The species entropy denotes the basal-area-weighted Shannon entropy in the forest stands.

S4 Computation of the basal-area-weighted DBH entropy

In the main text, we used the basal-area-weighted DBH entropy S_{DBH} (Fischer et al., 2024) as a measure for structural diversity. Specifically, this quantity measures the diversity of DBH values in a forest stand taking into account that the ecological effect of large trees is much higher than that of small trees. The basal-area-weighted DBH entropy is computed as follows:

$$S_{\text{DBH}} = - \int_0^{\infty} f_d(\delta) \ln f_d(\delta) d\delta, \quad (\text{S16})$$

where $f_d(\delta)$ is the estimated probability density of finding trees with DBH δ in the stand, weighted by basal areas. Following Fischer et al. (2024), we estimated $f_d(\delta)$ using a kernel-density estimation (see e.g. Wand and Jones, 1995):

$$f_d(\delta) = \sum_{d \in D} w_d K(d, \delta; h). \quad (\text{S17})$$

Here, D contains the DBH values of all trees in the forest patch (including repetitions if applicable), and

$$K(d, \delta; h) = \begin{cases} \frac{3}{4h} \left(1 - \left(\frac{d-\delta}{h}\right)^2\right) & \text{if } |d - \delta| \leq h \\ 0 & \text{else} \end{cases}$$

is the Epanechnikov kernel with bandwidth $h = 1$ cm, which measures how similar two DBH values are considered. DBH values d and δ with $|d - \delta| \geq h$ are considered completely dissimilar. The weights

$$w_d = \frac{d^2}{\sum_{d \in D} d^2} \quad (\text{S18})$$

express the individual trees weights according to their respective basal areas.

For a more in-depth discussion of the basal-area-weighted DBH entropy refer to Fischer et al. (2024) and its supplement.

S5 Updates to the parameterization of FORMIND for temperate forests

In this supplement, we provide the temperate forest parameterization of the forest model FORMIND that we used to simulate a large dataset of forest stands. We derived the parameterization from the work of Bohn et al. (2014), but adjusted it to (1) better reflect forest dynamics in structurally heterogeneous forests and (2) match the environmental conditions found at the Hohes Holz site used for the parameterization. To parameterize the model, we used allometric data from the Tallo database (Jucker et al., 2022), forest inventory data from the Hohes Holz site (10 ha), soil-type-specific values for hydrological parameters (Maidment, 1993), and unpublished soil and LAI data obtained on site. The Hohes Holz site is a mixed deciduous / evergreen ICOS forest site located in central northern Germany (mean ann. temperature 10.4°C; mean ann. precipitation 5171/m²; Holtmann et al., 2021).

We sought to minimize changes of the original parameterization where possible. Hence we focus on presenting the changes to the original parameterization and do not provide further details on FORMIND or the work by Bohn et al. (2014). We begin by providing an overview of the parameterization approach and the changes we introduced, then we provide details on individual steps where necessary. Finally, we provide a brief analysis of the dynamics of the updated model.

S5.1 Overview

S5.1.1 General approach

When updating the FORMIND parameterization for temperate forests (here: Hohes Holz site), we sought to satisfy the following criteria:

1. Agreement with field data.

- 240 – The allometric equations and the representation of environmental conditions should match observations from inventory and eddy flux field data.
- The mean LAI computed based on the forest inventory should match the independent on-site LAI estimate from the Hohes Holz site.
- 245 – Productivity and respiration should be parameterized so that for most of the trees in the inventory, the gross primary production (GPP) exceeds the respiratory needs for maintenance (see Fischer et al., 2024).

2. Consistency with first principles.

- The maintenance respiration of trees should increase monotonously with the tree size.
- Temporal upscaling of reference environmental conditions should be conducted consistently.

3. Consistency with expectations on long-term dynamics.

- 250 – The forest succession should yield a “reasonable” forest trajectory.

Besides satisfying these criteria, we also enabled model features that were developed after the initial work by Bohn et al. (2014) and improve the model’s mechanistic realism. Nonetheless, we pursued to limit the changes of the parameterization to the necessary minimum so as to facilitate consistency with previous work.

S5.1.2 Overview of changes

- 255 The allometric relationships for tree height, biomass, and crown diameter were fitted based on data from the Tallo database (Jucker et al., 2022). Then the LAI was adjusted, ensuring that (1) the mean LAI of the Hohes Holz forest matched an independent estimate and (2) the maintenance respiration is monotonously increasing with tree size. The balance between trees’ maintenance respiration and other carbon losses (e.g. growth respiration) was fitted by constraining the maintenance respiration based on the estimated productivity of trees in the Hohes Holz forest stand. Finally, the mortality was adjusted based on
- 260 simulations of the forest succession.

We enabled the defoliation mechanism (first introduced by Fischer et al., 2024) as a consistent way to account for trees whose respiratory needs exceed their gross primary productivity (GPP). To keep the overall mortality consistent with field data, we reduced the stochastic background mortality. Furthermore, we enabled a regeneration mechanism based on the available light. Lastly, we adjusted the soil and weather parameters based on the conditions found at the Hohes Holz site, and we adjusted the

265 climatic reference conditions that FORMIND uses to infer maintenance respiration based on the updated parameterization.

S5.2 Details

Below we provide further details regarding individual parameterization steps. The order of the sections reflects the execution order of the steps, as some parameterization results depend on one another.

S5.2.1 DBH-height relationships

- 270 To fit the DBH-height relationships, we used allometry data from the Tallo database (Jucker et al., 2022). This dataset contains more than 5,000 observations for Picea and Fagus, about 1,000 for Fraxinus and Betula, 643 and 445 for Quercus and Populus, respectively, and 18 for Robinia.

We assumed that the height is log-normally distributed around the mean, which is used in the model. This allowed us to fit the DBH-height relationship via an ordinary least squares fit on log-transformed data. We tested different functional relationships

	Pinus	Picea	Fagus	Quercus	Populus	Fraxinus	Betula	Robinia
h_0 [m]	81.1	61.46	124.08	57.05	48.51	57.23	56.63	66.91
h_1 [m ^{h_2}]	0.93	0.39	1.8	0.46	10 ⁵	0.35	10 ⁵	10 ⁵
h_2 [–]	0.85	1.15	0.67	1.	0.62	1.	0.66	0.7

Table S2. Adjusted parameters for the DBH-height relationships.

275 between DBH and height:

$$h(d) = h_0 d^{h_1}, \quad (\text{S19})$$

$$h(d) = \frac{h_0 d}{h_1 + d}. \quad (\text{S20})$$

We found that each of the functional forms is optimal for some of the considered genera. Hence, we introduced a new, generalized relationship:

$$280 \quad h(d) = \frac{\tilde{h}_0 d^{\tilde{h}_2}}{\tilde{h}_1 + d^{\tilde{h}_2}}. \quad (\text{S21})$$

We applied the AIC criterion (Akaike, 1974) to determine whether to use one of the simpler models (S19) or (S20), or the joint model. Where model (S19) was optimal, we used the joint (S21) model with parameters $\tilde{h}_0 = 10^5 h_0$, $\tilde{h}_1 = 10^5$, and $\tilde{h}_2 = h_1$ after fitting the parameters of model (S19). This is an approximation to the limit of $\tilde{h}_0, \tilde{h}_1 \rightarrow \infty$, $\frac{\tilde{h}_0}{\tilde{h}_1} \rightarrow h_0$, where model (S21) reduces to model (S19). Only for populus, we manually chose model (S19) instead of model (S21), because (a) the latter would
285 have implied that trees need an excessively large DBH to reach their maximal height and (b) the difference in AIC between the models was small, justifying the choice of the simpler model ($\Delta\text{AIC} < 10$).

We chose model (S19) for the following genera: Populus, Betula, and Robinia. We chose model (S20) for Quercus and Fraxinus, and model (S21) for Pinus, Picea, and Fagus. The resulting parameters are displayed in Table S2, and the resulting curves, compared to the original DBH-height-relationships, are displayed in Fig. S2.

290 S5.2.2 DBH-biomass relationships

The stem biomass can be computed from the DBH based on rather simple geometrical assumptions and therefore with relatively high credibility. It is therefore a sensible tool to check the consistency of direct biomass estimates that were derived based on data not covering the entire range of possible trees sizes. Moreover, in the updated parameterization, the crown biomass (= total biomass – stem biomass) is also used to estimate how much crown damage a tree can tolerate before dying. Therefore,
295 we sought DBH-biomass relationships where stem biomass and total biomass were consistent with one another.

To enforce such a consistent parameterization of stem biomass and tree biomass, we assumed that the stem biomass is always at least 90% of the tree biomass. That is,

$$B(d) = \max\left(B_0(d), \frac{1}{0.9} B_s(d)\right), \quad (\text{S22})$$

where B is the total tree biomass,

$$300 \quad B_0(d) = \exp\left(\frac{b_0 (\ln(d \cdot C) - b_2) (2b_1 + \ln(d \cdot C) - b_2)}{b_1 + \ln(d \cdot C) - b_2}\right) [\text{t ODM}] \quad (\text{S23})$$

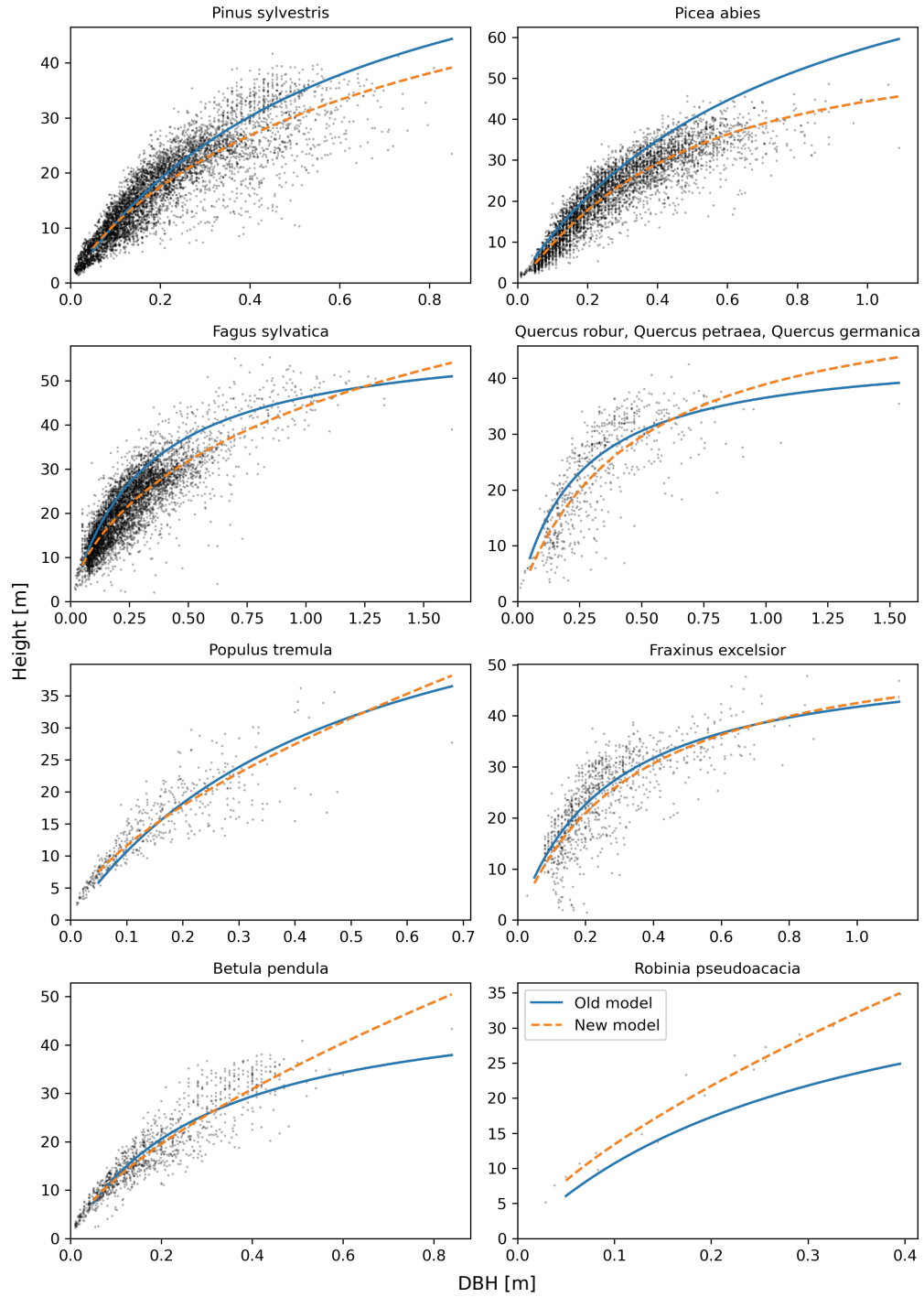


Figure S2. DBH-height relationships for the considered species / genera. The black dots display the data from the Tallo database (Jucker et al., 2022); the solid blue curves show the relationships as they were in the old parameterization, whereas the dashed orange lines show the newly fitted curves.

	Pinus	Picea	Fagus	Quercus	Populus	Fraxinus	Betula	Robinia
b_0 [—]	1.202	1.213	1.180	1.232	1.363	1.237	1.227	1.389
b_1 [—]	7222.6	78.61	15395	7802	5542	34929	5391.9	7213.9
b_2 [—]	3.675	3.679	3.474	3.575	3.795	3.530	3.631	3.497

Table S3. Adjusted parameters for the DBH-biomass relationships.

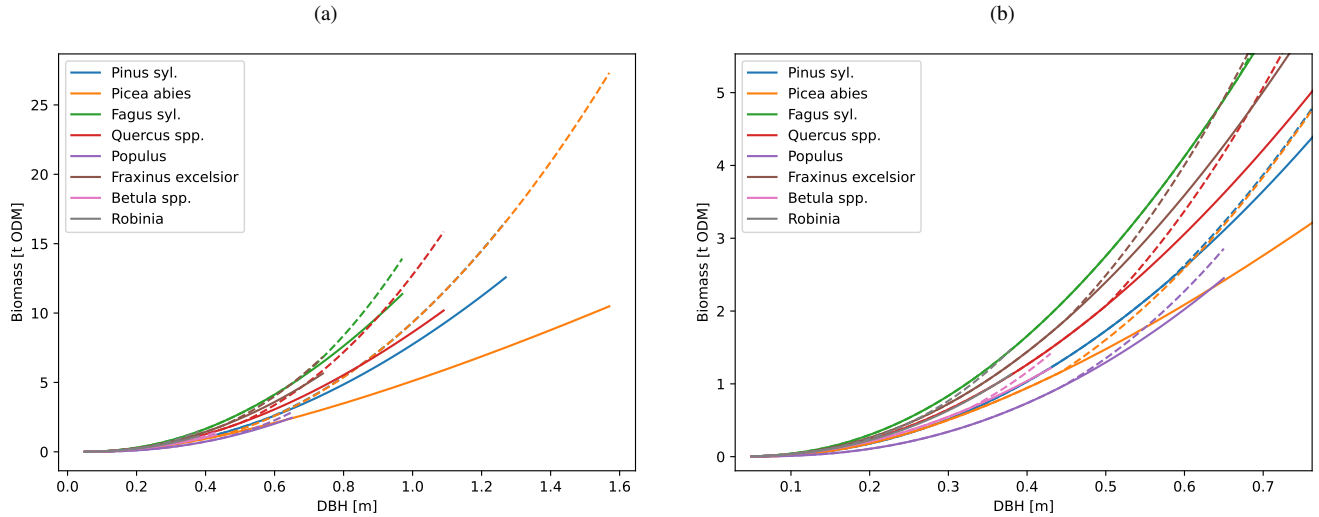


Figure S3. Comparison of the new and old DBH-biomass relationships for the different considered genera. The solid lines depict the relationships as they were in the old parameterization (or $B_0(d)$); the dashed lines show the adjusted relationships (or $B(d)$). Note that the original biomass equations were fitted to data that only included trees of 0.27 m–0.75 m DBH, where the curves still match relatively well.

with conversion factor $C = 100 \frac{1}{\text{m}}$ is the tree biomass equation derived by Bohn et al. (2014) based on data by Schober (1995), and B_s is the stem biomass computed based on tree geometry and allometric equations.

The resulting curves in comparison to the curves by Bohn et al. (2014) are depicted in Fig. S3. Especially for large trees, the differences are significant. Note, however, that the data by Schober (1995) often only include stands with mean DBH of up to 0.75 m (Pinus: 0.43 m, Spruce: 0.44 m, Fagus: 0.54 m, Quercus: 0.70 m, Populus: 0.75 m, Fraxinus: 0.31 m, Betula: 0.27 m, Robinia: 0.41 m). Within this range, the differences between original and updated parameterization are moderate.

Equation (S22) is not differentiable everywhere, leading to discontinuities in the maintenance respiration calculation. Hence, we fitted adjusted biomass curves of form (S23) to the joint equation (S22). Here, we minimized the absolute error between the new curves and $B(d)$ in the interval between the minimal and the maximal DBH of each genus. The resulting curves matched $B(d)$ well. The new parameters are shown in Table S3.

	Pinus	Picea	Fagus	Quercus	Populus	Fraxinus	Betula	Robinia
$d_0[\text{m}]$	0.557	1.32	2.45	1.22	1.11	0.998	0.786	1.73
$d_1 [-]$	12.3	10.1	13.8	15.8	13.7	13.4	18.4	9.19

Table S4. Adjusted parameters for the DBH-crown-diameter relationships.

S5.2.3 DBH-crown-diameter relationships

We refitted the DBH-crown-diameter relationships using the same approach described in section S2. After an initial investigation, we chose to change the relationship to a simple affine-linear model $D_c(d) = d_0 + d_1 d$, which often also matched the data better. The resulting parameters are provided in Table S4, and the resulting changes are displayed in Fig. S4.

315 S5.2.4 DBH-LAI relationships

We adjusted the trees' LAI values to approximately match the overall mean value of 3.5 roughly estimated based on LIDAR measurements for the Hohes Holz site (unpublished data). Before the adjustment, the LAI was larger than 5 in the forest area. We adjusted the LAI values for all genera proportionally until we obtained the desired mean value for the forest area. We achieved that by multiplying the LAI values by a factor of about 0.75. Only for Robinia, we kept the original value of 5, as the low maintenance respiration resulting from a small LAI would otherwise have lead to a dominance of this species in simulations of the forest succession.

An analysis of the growth of small individuals revealed that they used a high fraction of their GPP for maintenance respiration (Fig S5). Hence, subtle shading by major trees led to the death of these plants, hindering the regeneration of the forest. Furthermore, the fraction of GPP used for maintenance decreased with tree sizes, which disagrees with theoretical results suggesting that the fraction of GPP used for maintenance should monotonously increase with tree size.

We solved this issue by reducing the LAI for small trees. Due to FORMIND's "inverse" approach to estimate the maintenance respiration based on reference climate conditions, the maintenance respiration is positively related to the LAI. We manually adjusted the DBH-LAI relationship until the fraction of GPP used for maintenance increased monotonously. To that end, we used a piece-wise linear ansatz for the relationship:

$$330 \quad L(d) = \begin{cases} l_0 + (d - \bar{d}_0) \frac{l_1 - l_0}{\bar{d}_1 - \bar{d}_0} & \text{if } \bar{d}_0 \leq d < \bar{d}_1 \\ l_1 + (d - \bar{d}_1) \frac{l_2 - l_1}{\bar{d}_2 - \bar{d}_1} & \text{if } \bar{d}_1 \leq d < \bar{d}_2 \\ l_2 & \text{if } \bar{d}_2 \leq d, \end{cases} \quad (\text{S24})$$

where L denotes the LAI, l_0 , l_1 , l_2 are minimal, intermediate, and final LAI value, respectively, $\bar{d}_0$ is the initial DBH of seedlings, and $\bar{d}_1$ and $\bar{d}_2$ are the DBH values where the intermediate and the final LAI are attained, respectively. The changes affected small trees only and did not decrease the overall LAI of the Hohes Holz forest significantly. The chosen parameters are displayed in Table S5; the resulting LAI and respiration curves are depicted in Fig. S5.

335 S5.2.5 Maximal height for Robinia

We changed the maximal height for Robinia from 27.3m to 34m. Without this adjustment, the maximal height would have corresponded to a relatively small maximal diameter at breast height (DBH) according to the new height-stem-diameter relationship. As FORMIND uses the DBH as central measure for tree size internally, the small maximal diameter would have limited tree growth very early. The new height maximum was determined based on the Tallo database (Jucker et al., 2022).

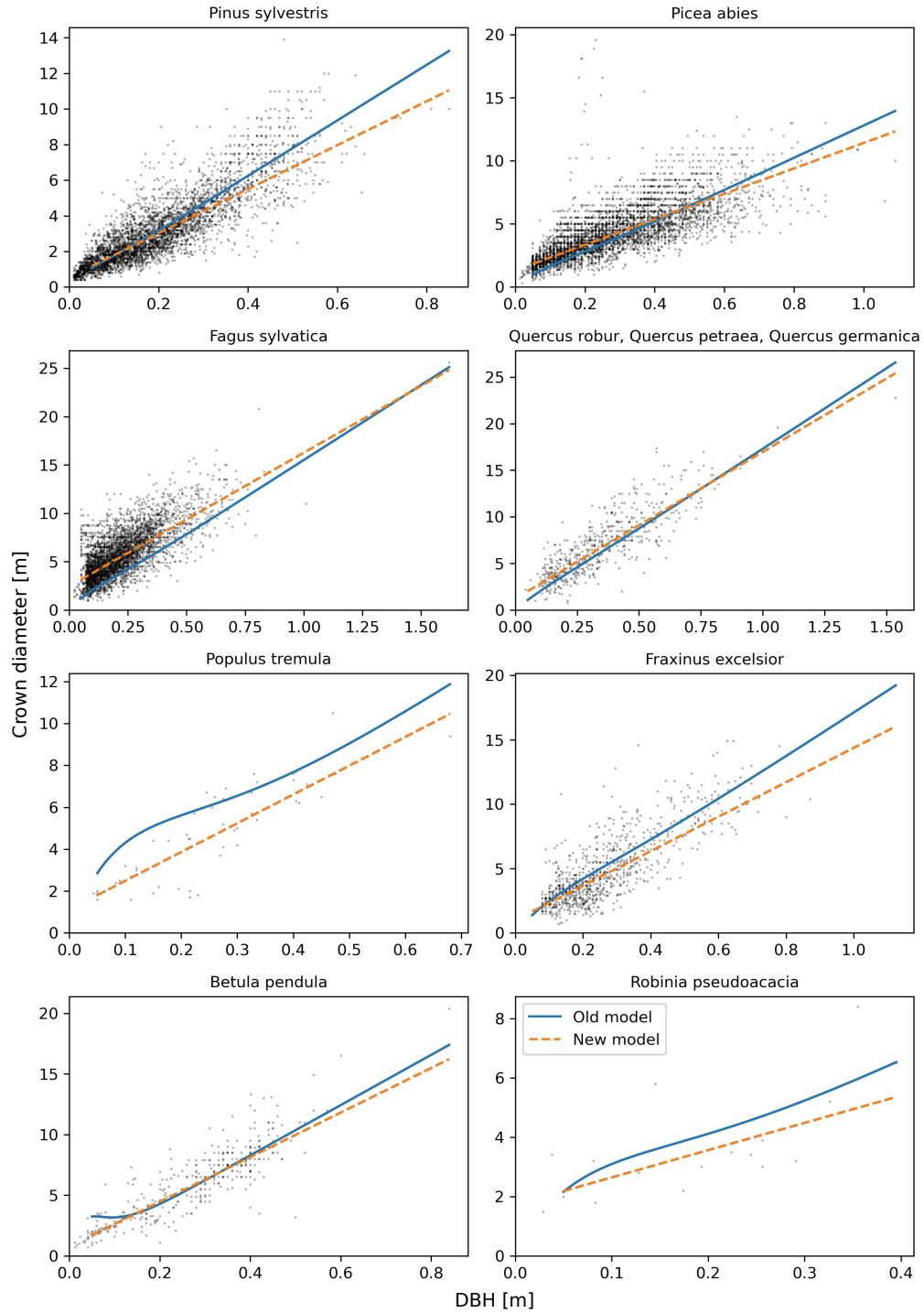


Figure S4. DBH-crown-diameter relationships for the considered species / genera. The black dots display the data from the Tallo database (Jucker et al., 2022); the solid blue curves show the relationships as they were in the old parameterization, whereas the dashed orange lines show the newly fitted curves.

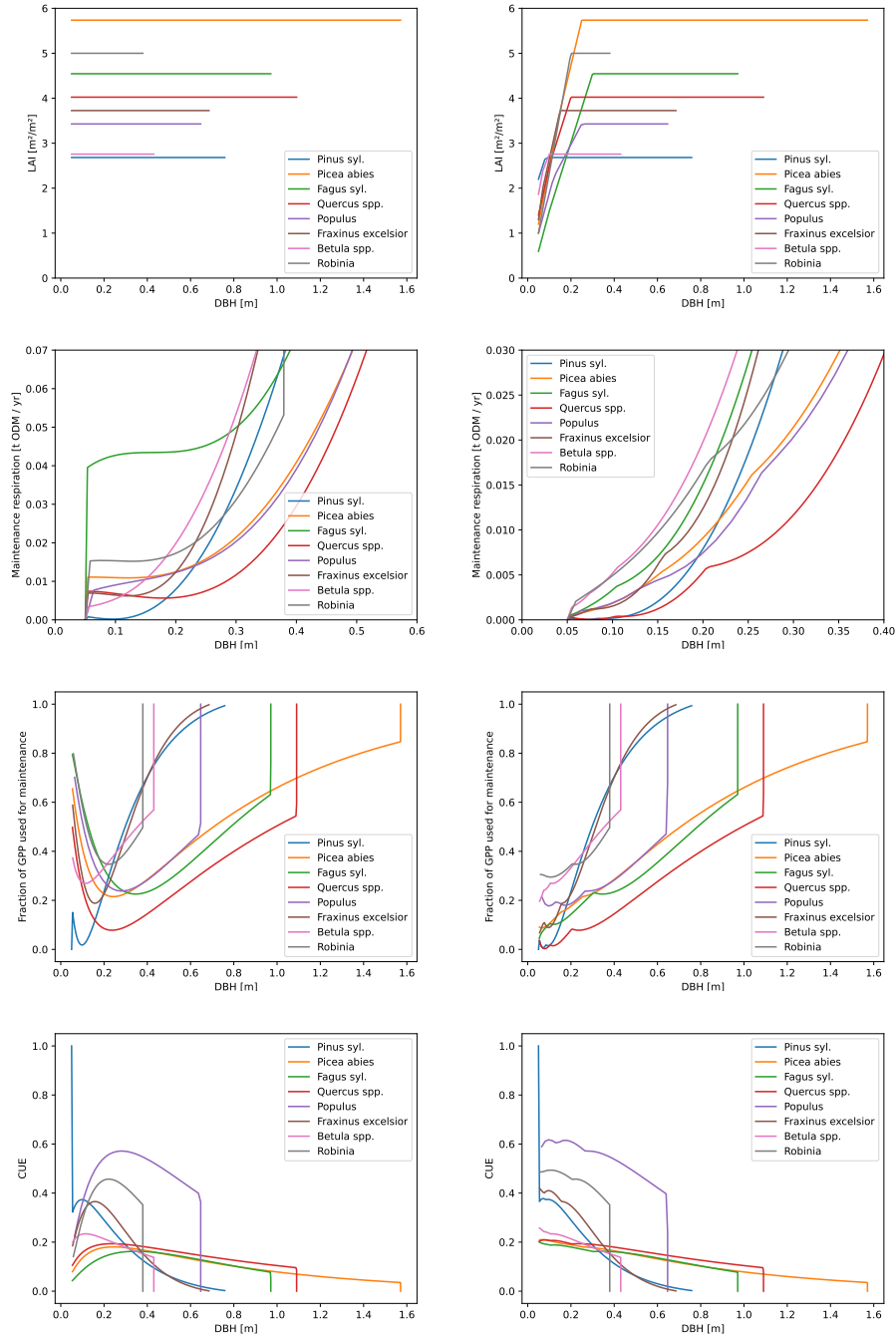


Figure S5. Impact of the LAI on carbon usage. All figures were created with the same parameterization except that the LAI was kept constant in the left figures, whereas it was adjusted in the right figures. If the LAI is kept constant, the maintenance respiration of small trees is high, leading to an initial decrease in the fraction of the GPP required for maintenance.

	Pinus	Picea	Fagus	Quercus	Populus	Fraxinus	Betula	Robinia
$\bar{d}_0$ [m]	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
$\bar{d}_1$ [m]	0.08	0.15	0.1	0.1	0.12	0.07	0.07	0.2
$\bar{d}_2$ [m]	0.1	0.25	0.3	0.2	0.25	0.15	0.1	0.2
l_0 [–]	2.2	1.2	0.596	1.4	1	1.3	1.863	1
l_1 [–]	2.65	3.726	1.49	2.5	2.235	2	2.384	5
l_2 [–]	2.682	5.737	4.545	4.024	3.428	3.726	2.757	5

Table S5. Adjusted parameters for the DBH-LAI relationships.

340 S5.2.6 Light extinction coefficient

We reduced the light extinction coefficient from 0.7 to 0.5. This parameter change increases the potential forest density and is in line with common radiative transfer model parameterizations (Yang et al., 2017) and the parameterization by Fischer et al. (2024).

S5.2.7 Soil and weather parameters

345 We adjusted the soil and weather parameters based on the conditions found at the Hohes Holz site.

- The initial soil water content was set to a value of 21 % (v/v) so that the soil water content does not change significantly over time (i.e., directly hits its equilibrium) at the Hohes Holz site.
- The mean rainfall duration for rainy days was reduced from $24 \frac{\text{h}}{\text{day}}$ to a value of $6 \frac{\text{h}}{\text{day}}$.
- The soil rooting depth was reduced from 20 m to 2 m, which reflects the soil conditions at the Hohes Holz site.
- 350 – The permanent wilting point was adjusted from 20.8 % to 13.3 % according to Maidment (1993) p. 5.14 (silt loam soil; water retained at -1500 kPa).
- The field capacity was changed from 36.6 % to 33 % according to Maidment (1993) p. 5.14 (silt loam soil; water retained at -33 kPa).
- The soil porosity was increased from 46.3 % to 50.1 % according to field measurements at the Hohes Holz site. An identical value is shown in Maidment (1993) p. 5.14 (silt loam soil).
- 355 – The fully saturated conductivity was adjusted from a value of $3.66 \cdot 10^{-6} \frac{\text{m}}{\text{s}}$ to $6.944 \cdot 10^{-7} \frac{\text{m}}{\text{s}}$ according to the value displayed in Fig. 5.3.3 on p. 5.16 in Maidment (1993); value estimated for 7.6 % sand, 14.9 % clay, and 77.5 % silt (soil composition of Hohes Holz).
- The pore size distribution index was set from 0.252 to 0.234 according to Maidment (1993) p. 5.14 (silt loam soil).
- 360 – The residual soil water content was reduced from 2.7 to 1.5 according to Maidment (1993) p. 5.14 (silt loam soil).

	Pinus	Picea	Fagus	Quercus	Populus	Fraxinus	Betula	Robinia
Ref. irradiance $\left[\frac{\mu\text{Mol photon}}{\text{m}^2 \cdot \text{s}} \right]$	553.760	552.686	893.750	833.594	842.188	893.750	833.594	842.188
Ref. GPP reduction $[-]$	0.798	0.788	0.802	0.806	0.853	0.844	0.800	0.865

Table S6. Adjusted parameters for reference climatic conditions.

S5.2.8 Climatic reference conditions

The climatic reference conditions denote the growth conditions of an unshaded tree within a forest with typical climate. The reference conditions are needed to compute the maintenance respiration of trees by comparing the GPP of a tree under reference conditions with the observed growth of such a tree. The carbon difference between GPP and observed wood production is assumed to be used for respiration and other losses.

For performance reasons, the GPP of the tree under reference conditions is computed under “mean” conditions for an entire year rather than on a daily resolution. Since several model processes are non-linear, the reference conditions (e.g. reference irradiation) are not simply given by a yearly mean (e.g. mean yearly irradiance) but need to be determined via a more intricate approach. Here, the goal is to achieve that a reference tree simulated with yearly time step has approximately the same GPP, NPP, and respiration as a tree simulated under the same conditions but on a daily resolution. This goal also drove our general approach: we considered two trees x_0 and x_1 simulated with a yearly and a daily time step, respectively, and adjusted the property in question (e.g. the irradiance) of x_0 until its GPP and NPP matched the one of tree x_1 .

Below, we used a “mean” daily climate for the reference conditions. That is, we averaged the climate from the years 2000-2017 at a site (longitude 11.5, latitude 51.8) close to the Hohes Holz area (longitude 11.22, latitude 52.09) for each day of the year.

S5.2.9 Reference vegetation period length

We retrieved the length of the vegetation period directly by simulating the forest under reference conditions for one year with a daily step. The length of the vegetation period can be directly used in the simplified model version with yearly time step. We obtained a value of 0.57 yr for the mean vegetation period length.

S5.2.10 Reference irradiance

We considered a simple and an advanced model to estimate the reference irradiation, where the simple model used a constant irradiance and day length, corresponding to the respective averages in the vegetation period, whereas the advanced model considered day length and irradiance on a daily basis. For each genus, we considered an individual with a DBH half as big as its maximal DBH and adjusted the mean incoming irradiance of the simple model until the GPP of the trees in the simple and the advanced model matched. Since the GPP scales linearly with day length, only one of mean irradiance and mean day length are identifiable, and we could set the mean day length to a value of 12h in the simple model without loss of accuracy.

Since the light response curves are genus-dependent, we obtained a different reference irradiance for each genus. In particular, the reference irradiance was lower for evergreen trees than for deciduous trees, as the latter do not grow in winter. The updated reference irradiance values can be found in Tab. S6.

S5.2.11 Reference GPP reduction

The reference GPP reduction specifies by how much the GPP of a tree under reference conditions is reduced by environmental factors. As water competition depends on all trees in a patch, we needed to consider reference trees with “usual” competition. We considered all $20\text{m} \times 20\text{m}$ patches with a biomass of at least $15\text{t ODM} = 375 \frac{\text{t ODM}}{\text{ha}}$ in the inventory and searched for

each genus an unshaded tree, which we then used as reference tree. For this tree, we determined the GPP with and without reduction by water competition and temperature effects. The desired reduction factor was the quotient of these two numbers.

If a genus was not present in the inventory, we identified the largest unshaded tree in the inventory with a DBH below the genus' maximal DBH and changed the selected tree's genus to the genus we wanted to consider. Then we used the selected tree as reference tree. The reference GPP reduction factors are displayed in Tab. S6.

S5.2.12 Respiratory losses

To determine the extent of trees' carbon losses not required for maintenance, we applied the approach proposed by Fischer et al. (2024). Based on the light climate, we determined for each tree in the forest the maximal maintenance respiration that the tree could satisfy with his GPP at its location, assuming that

$$\text{GPP} \geq \text{maintenance respiration.} \quad (\text{S25})$$

This formula should hold for most trees in general, but due to model simplifications (e.g., discretization of space), some trees observed in the inventory may not satisfy this condition for GPP and maintenance respiration computed with FORMIND.

In FORMIND, the carbon balance of each tree is closed, i.e.,

$$\text{GPP} = \text{NPP} + \text{maintenance respiration} + \text{other losses,} \quad (\text{S26})$$

where NPP and the loss term are proportional:

$$\text{other losses} = \frac{\gamma}{1 - \gamma} \text{NPP,}$$

so that we can write

$$\text{NPP} = (1 - \gamma) (\text{GPP} - \text{maintenance respiration}), \quad (\text{S27})$$

or equivalently

$$\text{maintenance respiration} = \text{GPP} - \frac{\text{NPP}}{1 - \gamma}, \quad (\text{S28})$$

where γ is the loss factor. As equation (S28) holds in particular for trees under reference conditions, whose NPP is known, the maintenance respiration is directly related to γ , and a change in γ impacts how many trees in the inventory satisfy inequality (S25). We identified the value of γ , where (S25) holds for 90% of the trees at Hohes Holz. If we considered each genus independently, the following values for the loss fraction would be required: Pinus: 0.63, Picea: 0.72, Fagus: 0.77, Quercus: 0.71, Betula: 0.74. If we considered all individuals simultaneously, a value of 0.77 would be necessary.

We used these growth loss factors γ as basis for the parameterization but adjusted them based on follow-up considerations. For Pinus, the GPP under reference conditions was not high enough to support 63% losses for trees of certain sizes. That is, the maintenance respiration was typically small enough to satisfy inequality (S25), but for small trees, we observed that $(1 - \gamma)\text{GPP} < \text{NPP}$ under reference conditions. Therefore, we reduced the loss value to $\gamma = 0.62$. For Picea, Fagus, and for Quercus, we increased the loss values so as to allow for a sufficient density and diversity of forests in succession runs. For Betula, we decreased the loss value to prevent it from becoming the dominant species in succession runs.

We chose loss values for the genera not present in the Hohes Holz area by matching the other genera's fraction of GPP used for maintenance respiration (Fig. S5). However, Populus and Robinia had a very high carbon use efficiency, making them extremely competitive in simulations. Therefore, we set their growth loss fractions to smaller values (0.25 and 0.3, respectively), which match the values from earlier FORMIND parameterizations. This manual fine tuning was necessary due to a lack of data needed for a more rigorous approach. The final chosen values for γ are displayed in Table S7.

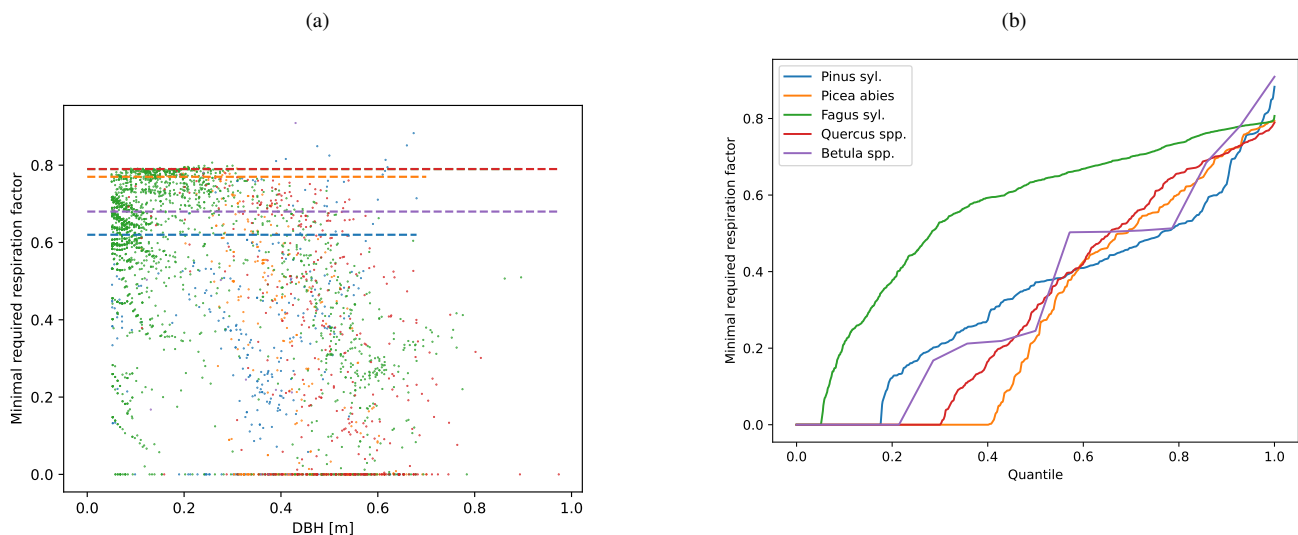


Figure S6. (a) Minimal required loss (here: “respiration”) factor γ required to satisfy inequality (S25) for each tree in the inventory. Each dot corresponds to a tree; the dashed lines correspond to the values of γ used in the parameterization. (b) Minimal respiration factor γ required to satisfy inequality (S25) for the given quantiles (fractions) of each genus’ individuals.

	Pinus	Picea	Fagus	Quercus	Populus	Fraxinus	Betula	Robinia
Respiration / loss factors [–]	0.62	0.77	0.79	0.79	0.25	0.55	0.68	0.3

Table S7. Adjusted respiration / loss factors.

430 S5.2.13 Mortality

We enabled the defoliation mechanism (first introduced by Fischer et al., 2024) as a consistent way to account for trees whose respiratory needs exceed their gross primary productivity (GPP). As both respiration and GPP depend on weather conditions and water supply, this mechanism also allows modelling the impact of climatic conditions (e.g. drought) on mortality. We disabled the earlier approach for handling trees whose respiration exceed their GPP, which had assigned such trees an increased stochastic mortality rate.

As trees could die due to loss of leafs after the aforementioned update, we reduced the DBH-dependent stochastic background mortality probabilities for all species by factor 0.705 in turn. This factor was chosen so that the forest biomass obtained in long succession runs matched the biomass in the inventory. The updated parameter values can be found in Table S8.

S5.2.14 Regeneration

440 The original parameterization by Bohn et al. (2014) did not consider regeneration. As no data for parameterizing ingrowth were available to us, we assumed that regeneration is not limited by the number of seeds but rather the available light. Hence, we set the number of in-growing saplings to a large number ($100 \frac{1}{\text{ha} \cdot \text{yr}}$).

	Pinus	Picea	Fagus	Quercus	Populus	Fraxinus	Betula	Robinia
Mortality scaling $a \left[\frac{1}{\text{yr}} \right]$	0.0027	0.0045	0.0062	0.0046	0.0119	0.0020	0.0129	0.0084
Mortality exponent $b [-]$	-1.271	-0.953	-0.761	-0.950	-0.894	-1.505	-0.210	-0.373

Table S8. Adjusted parameters for the DBH-dependent mortality function $\mathbb{P}(\text{death}) = a \cdot \text{DBH}^b$.

S5.3 Analysis of the new parameterization

445 With the adjusted parameterization, we obtained the following main characteristics of the Hohes Holz forest, initialized based on the inventory:

Biomass: $326.79 \frac{\text{t ODM}}{\text{ha}}$

Stem count: $214.61 \frac{1}{\text{ha}}$

Basal area: $27.49 \frac{\text{m}^2}{\text{ha}}$

LAI: 3.5

450 **GPP:** $34.46 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$ (2015: $32.9 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$ c.f. measured value of $38 \pm 3 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$; Pohl et al., 2023)

NPP: $4.17 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$ (2015: $3.70 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$ c.f. measured NEP value of $7 \pm 0.7 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$; Pohl et al., 2023)

Respiration: $34.29 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$ (2015: $29.19 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$ c.f. measured ecosystem respiration value of $31 \pm 3.6 \frac{\text{t ODM}}{\text{ha} \cdot \text{yr}}$; Pohl et al., 2023)

The reference values by Pohl et al. (2023) were measured via an on-site Eddy-flux tower.

455 Most of the main forest characteristics matched field estimates in their order of magnitude. Only the NPP was lower than expected, since the measured NEP value, which is a lower bound for NPP, is almost twice as big as the modelled NPP.

If the model is run from bare ground, FORMIND predicts the emergence of a beech-dominated forest at the Hohes Holz site (see Fig. S7). In the first 200 years, fast-growing genera (Populus and Robinia) dominate, but Betula always remains at a low density. After 400 years, the forest composition remains roughly constant. Conifers play a minor role; Quercus becomes the second-most abundant genus.

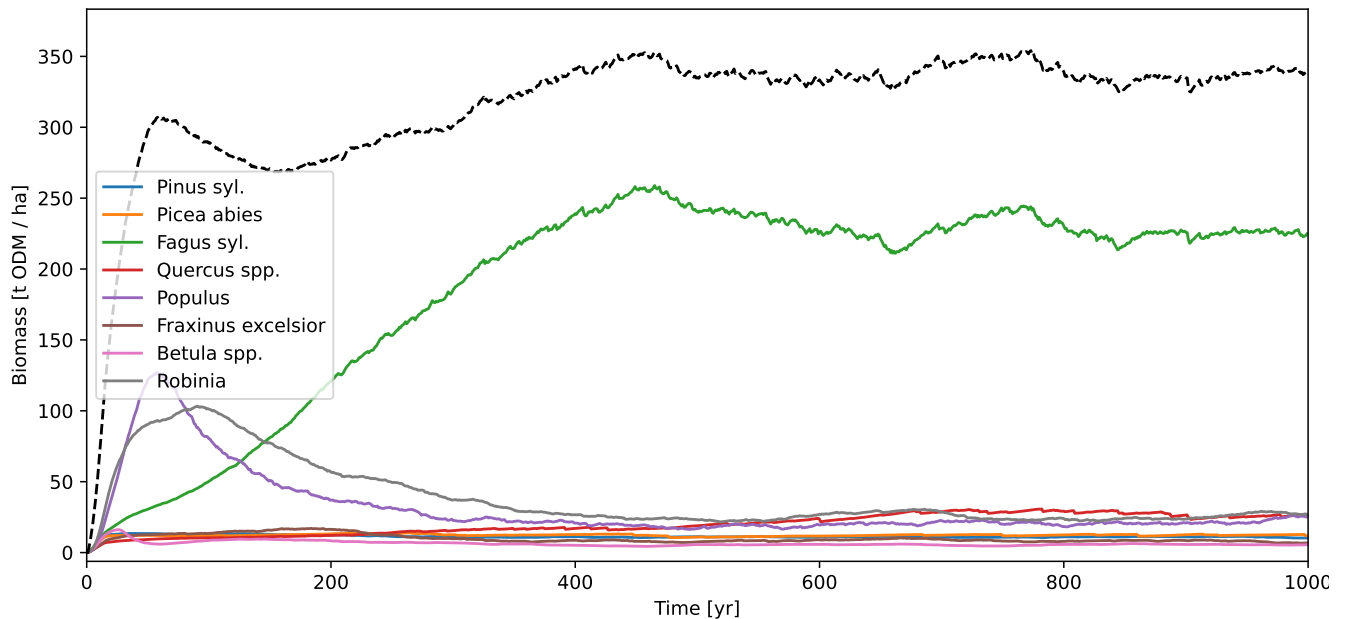


Figure S7. Succession of 8 ha forest under the climatic conditions of Hohes Holz (2000–2017). The dashed black line depicts the forest’s total biomass.

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