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Matching scales of eddy covariance measurements and process-based modeling – assessing spatiotemporal dynamics of carbon and water fluxes in a mixed forest in Southern Germany

Hassane Moutahir et al.

Correspondence to: Hassane Moutahir (hassane.moutahir@partner.kit.edu) and Rüdiger Grote (ruediger.grote@kit.edu)

Supplementary materials

Site selection for calibration and application of additional quality criteria

Model calibration was carried out with eddy-covariance data from various long-term field observatories equipped with an eddy-flux tower. For beech (*Fagus sylvatica*), three ICOS sites (Leinefelde in Germany (DE-Lnf), Soroe in Denmark (DK-Sor), and Stitna in the Czech Republic (CZ-Stn)), and for Douglas fir (*Pseudotsuga menziesii*), data from the Speulderbos site in the Netherlands and the ICOS site Campbell River in Canada (CA-Ca1) were used.

Quality filtering at all sites was applied using the available quality flags. Daily NEE values were only included when half-hourly data consisted of at least 70% measured or high-quality gap-filled values. Days not meeting this criterion were discarded to avoid bias from excessive gap-filling.

For the Speulderbos site, the flux data that showed substantial noise and thus were subjected to additional quality control prior to calibration and evaluation. It was found that ancillary gas concentration measurements required for the Webb-Pearman-Leuning (WPL) density correction were not consistently available at this site, resulting in a compromised density correction in periods with missing H_2O data and thus to further data exclusions.

In addition, tower-based meteorological observations were cross-checked against ERA5 reanalysis data to identify inconsistencies in climate forcing. At the Campbell River site, two years exhibiting persistent and substantial deviations between tower measurements and reanalysis data (2004 and 2006) were thus excluded to ensure physically consistent forcing conditions during model calibration and evaluation.

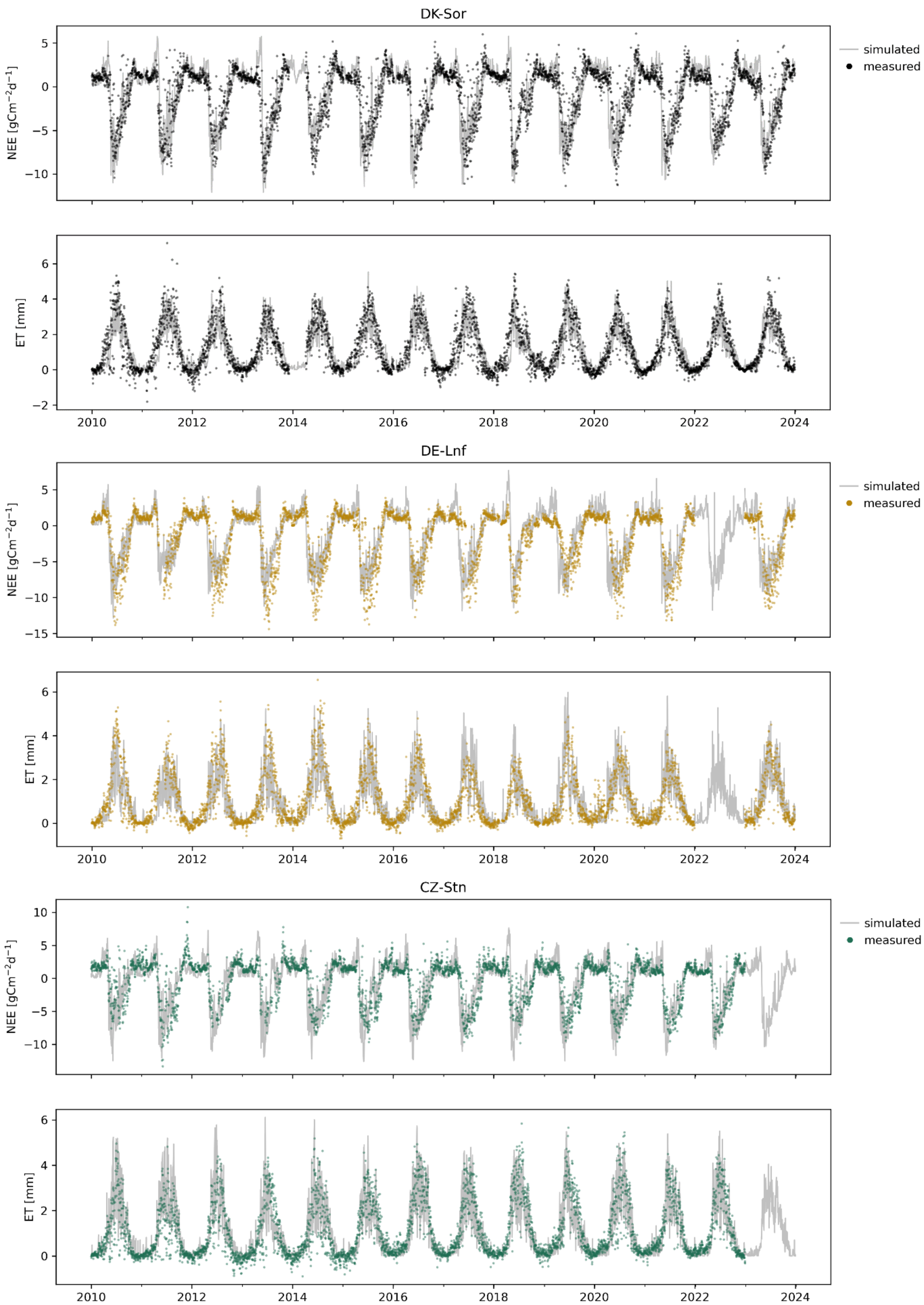

Fig. S1: Comparison of simulated (lines) and measured (dots) daily ecosystem fluxes at three beech sites (top: Soroe, DK, black dots; middle: Leinefelde, DE, yellow dots; bottom: Stitna, CZ, green dots) throughout the years 2010-2023. NEE: net carbon exchange (gC m^{-2} d^{-1}), ET: evapotranspiration (mm).

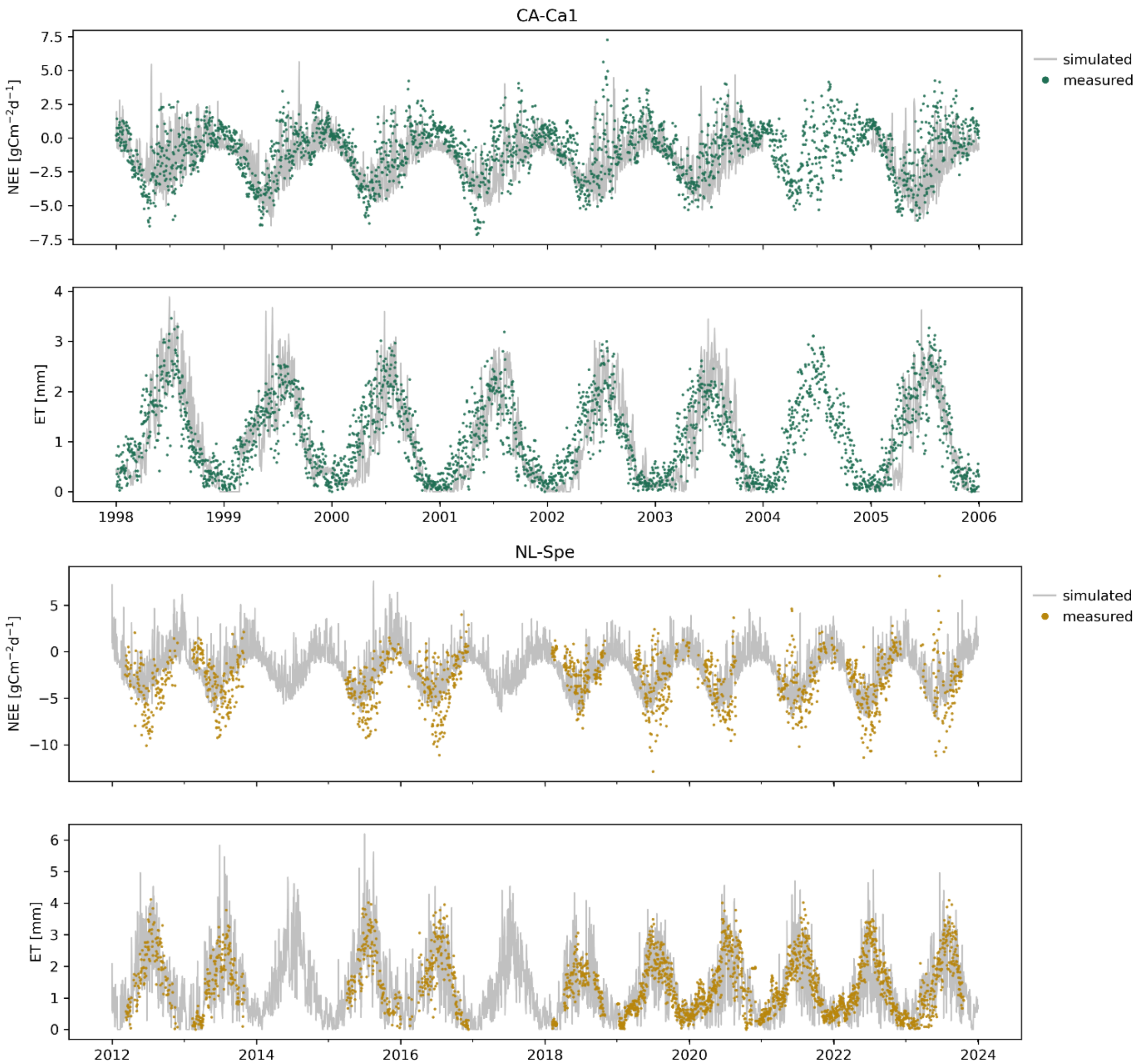

Fig. S2: Comparison of simulated (lines) and measured (dots) daily ecosystem fluxes at two Douglas fir sites (top: Campbell no1, CA, green dots; bottom: Speulderbos, NL, yellow dots) throughout the years 1998-2005 and 2012-2023, respectively. NEE: net ecosystem carbon exchange (gC m^{-2} d^{-1}), ET: evapotranspiration (mm).

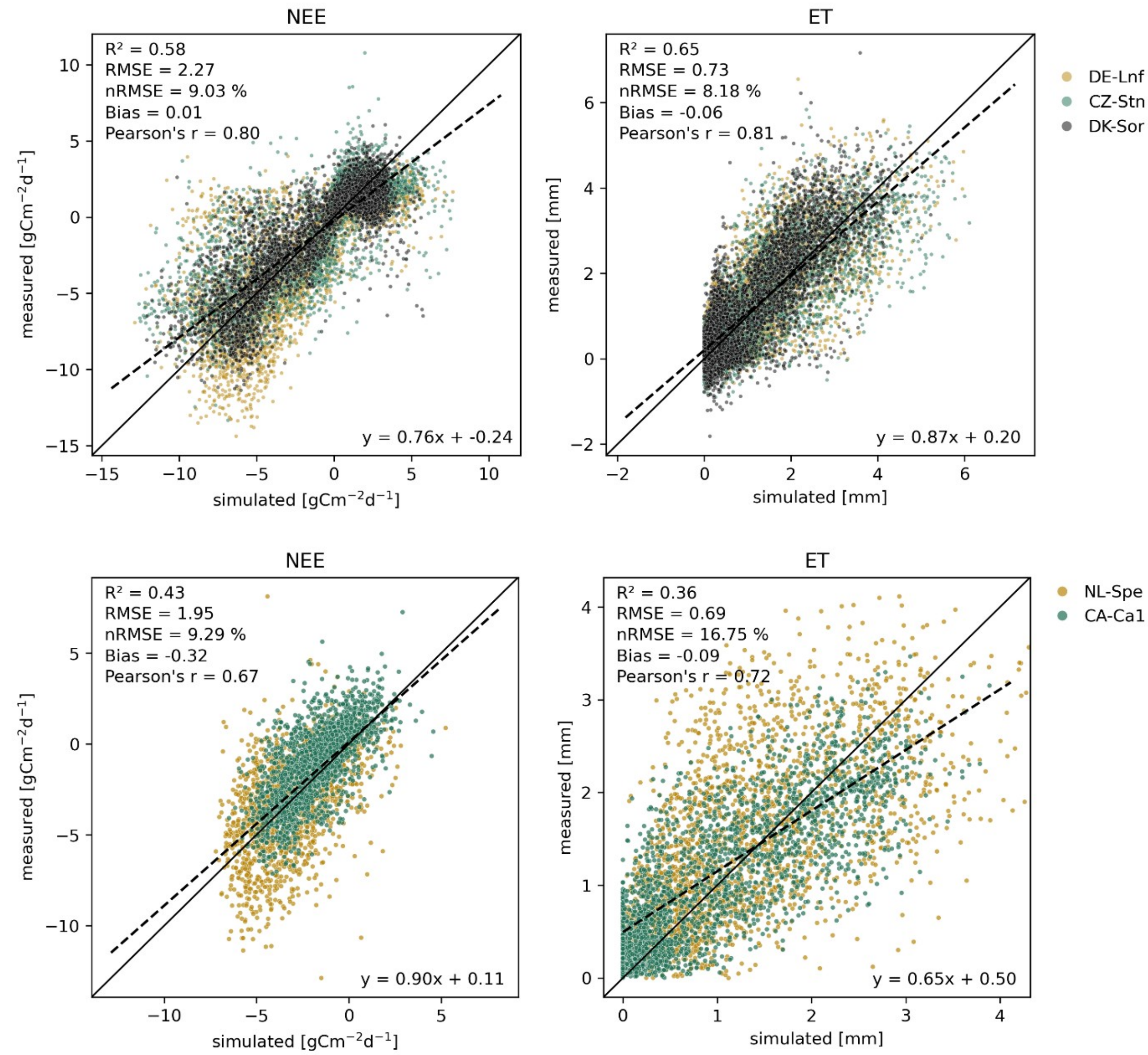

Fig. S3: Evaluation of simulated with measured daily ecosystem fluxes for all three Beech sites (top) and the two Douglas fir sites (bottom) for the whole investigation period. NEE (left): net ecosystem carbon exchange (gC m^{-2} d^{-1}), ET (right): evapotranspiration (mm). Different sites are depicted in different colors with the same color code as in Figures S1 and S2. Metrics include squared coefficient of determination (R^2), relative squared mean error (RSME), normalized relative squared mean error (nRSME), model bias (gC m^{-2} d^{-1} and mm, respectively), and Pearson's coefficient of determination (r).

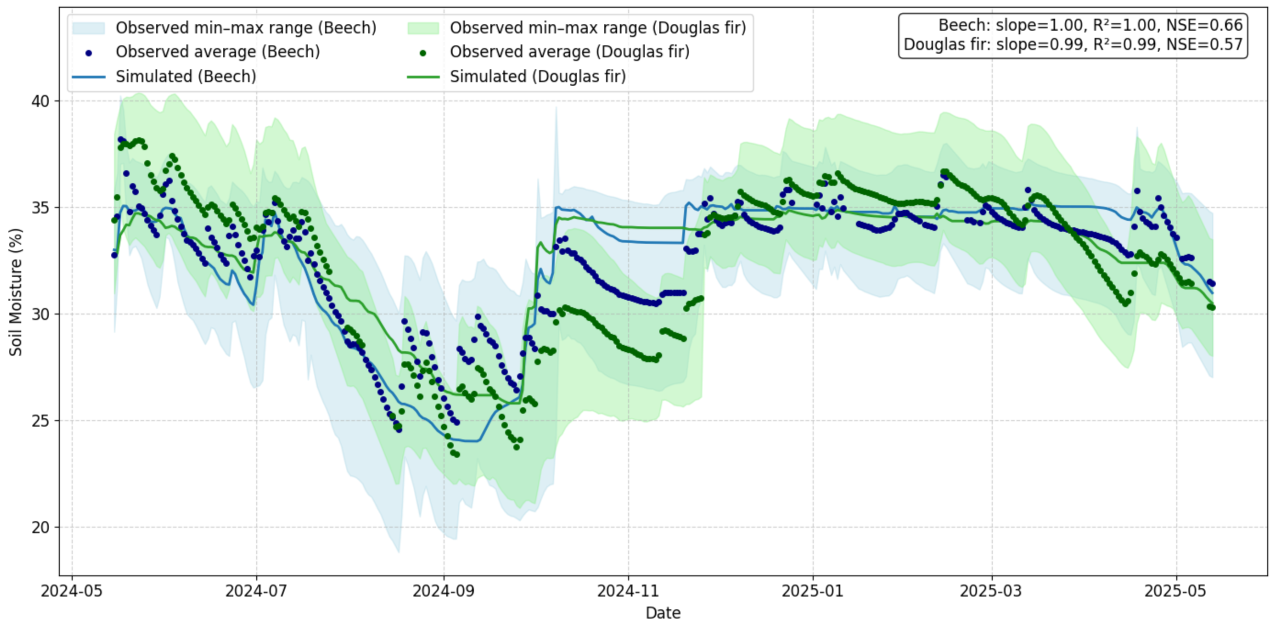

Fig. S4: Comparison of measured and simulated soil moisture at 50 cm depths in pure beech and pure Douglas fir plots from May 2024 to May 2025 at the ECOSENSE forest. Soil moisture was measured at five replicate points per depth in each plot. Simulated values are outputs of LandscapeDNDC model.

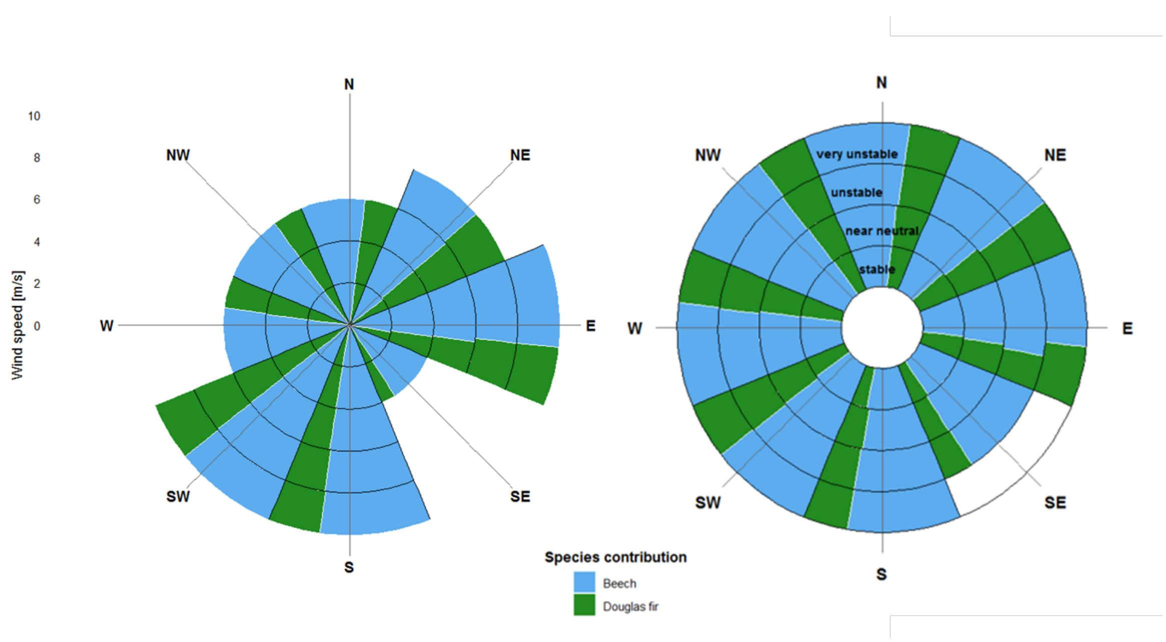

Fig. S5: Wind speed in different cardinal directions (left) and stability classes (right) both combined with species contribution from beech and Douglas fir, respectively. Four different stability classes were considered according to the stability parameter (ζ): very unstable ($\zeta \leq -1$), unstable ($-1 < \zeta \leq -0.1$), near-neutral ($-0.1 < \zeta \leq 0.1$), stable ($\zeta > 0.1$).

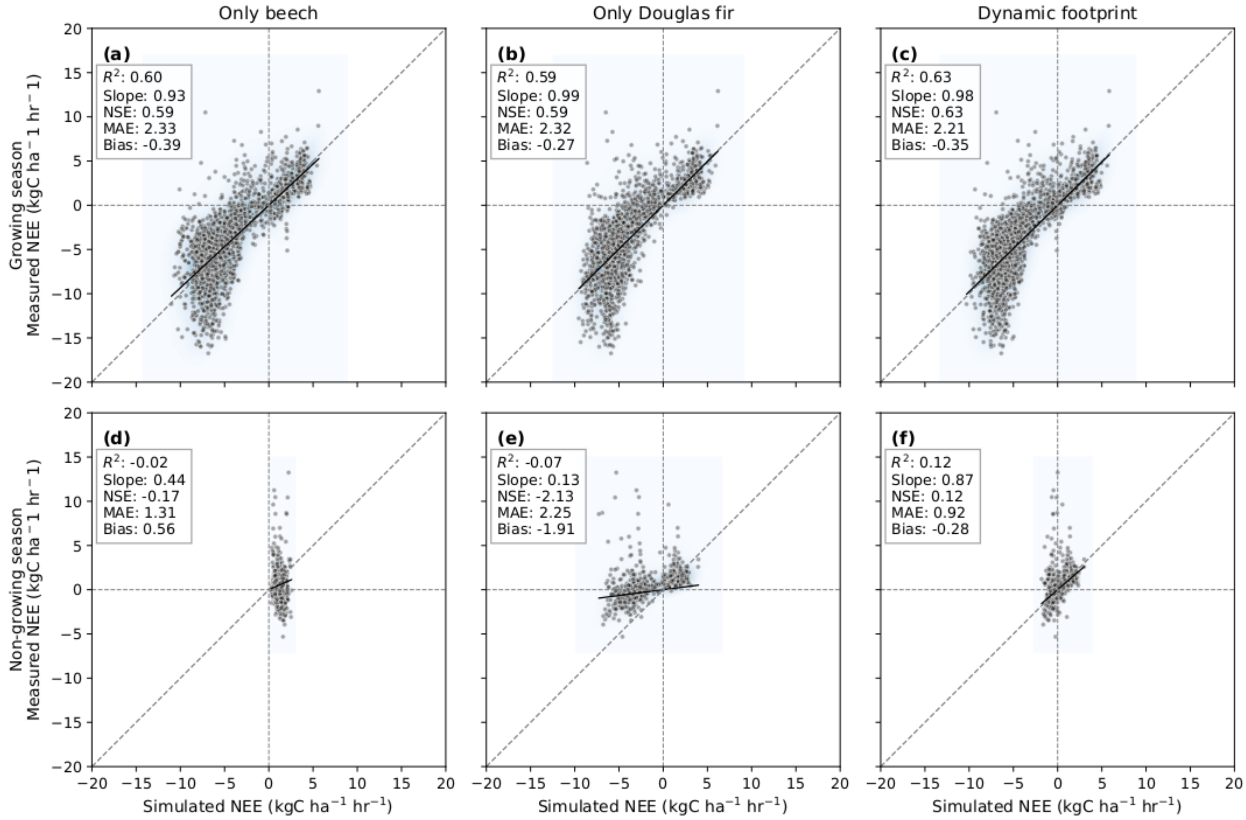

Fig. S6: Comparison between hourly measured and simulated net ecosystem carbon exchange (NEE, kgC ha^{-1} hr^{-1}) during the growing season (April – October) and non-growing season (November-March) at the ECOSENSE forest. (a and d) Simulated NEE for a pure beech stand compared to measured EC NEE. (b and e) Simulated NEE for a pure Douglas fir stand compared to measured EC NEE. (c and f) Weighted NEE based on a dynamic footprint composition, with hourly contributions from each species estimated using footprint–land cover overlay. The shaded heatmap represents the kernel density estimate of point concentrations (darker blue regions correspond to higher density).

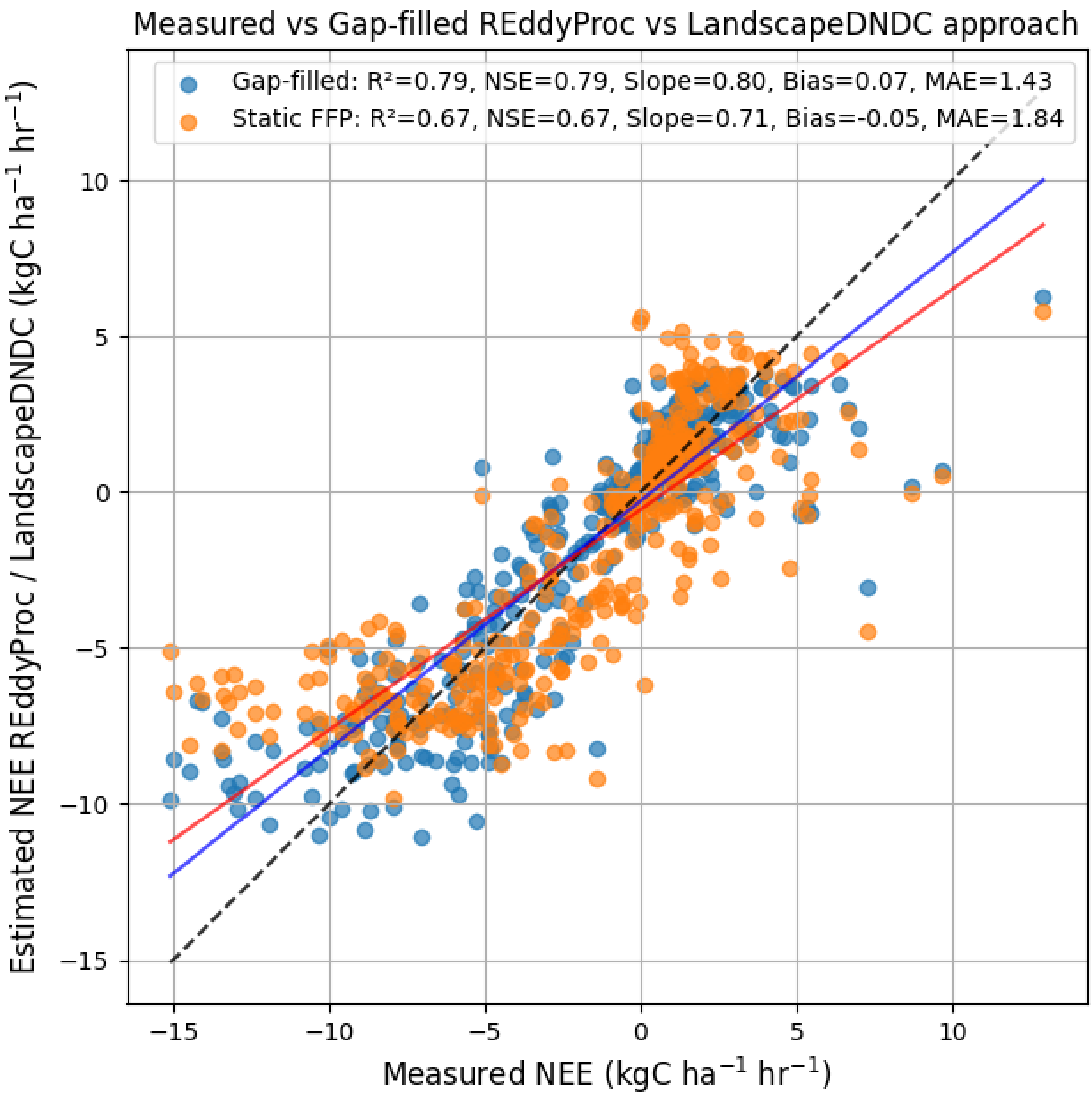

Fig. S7: Comparison between hourly measured and gap-filled net ecosystem carbon exchange (NEE, kgC ha^{-1} hr^{-1}) using the REddyProc (blue dots, labeled 'Gap-filled') and the process based LandscapeDNDC (orange dots, labeled 'Static FFP') approach. We randomly created 627 artificial gaps in the measured data and filled them with the two approaches.

Table S1: Parameters affecting the simulation of carbon and water exchange in the LandscapeDNDC model. Values are mostly taken from the literature but '*' indicate that they are calibrated within boundaries reported in the literature using specific sites.

Variable	Description	Beech	Douglas fir	References (Beech; Douglas fir)
Photosynthesis				
AEKC	Activation energy for Michaelis-Menten constant for CO_2 (J mol^{-1})	65000	65000	Wang et al. (2003); Falge et al. (1997) (assumed similar to Norway spruce)
AEKO	Activation energy for Michaelis-Menten constant for O_2 (J mol^{-1})	36000	36000	Wang et al. (2003); Falge et al. (1997) (assumed similar to Norway spruce)
AERD	Activation energy for dark respiration (J mol^{-1})	36500	63500	Dreyer et al. (2001); Falge et al. (1997) (assumed similar to Norway spruce)
AEVC	Activation energy for photosynthesis (J mol^{-1})	70627	75750	Kattge and Knorr (2007); Falge et al. (1997) (assumed similar to Norway spruce)
AEVO	Activation energy for RubP oxygenation (J mol^{-1})	37530	37530	Long (1991) (both species)
AEJM	Activation energy for electron transport (J mol^{-1})	48090	40000	Medlyn et al. (2002); Ibrom et al. (2006) (assumed similar to Norway spruce)
KC25	Michaelis-Menten constant for CO_2	299.5	260.0	Wang et al. (2003); Von Caemmerer et al. (1994)
KO25	Michaelis-Menten constant for O_2	159.6	179.0	Wang et al. (2003); Von Caemmerer et al. (1994)
QVOVC	Relation between saturated rate of oxygenation and carboxylation	0.21	0.21	Long (1991) (both species)
QJVC	Relation between max. electron transport rate and RubP-saturated carboxylation	2.24	2.8	Yan et al. (2023); Manter et al. (2003)
QRD25	Relation between dark respiration rate and carboxylation capacity	0.0149	0.012	Yan et al. (2023); Warren and Adams (2006)
SLOPE_GSA	Slope of stomata response in the BERRY-BALL model	11.8	4.0	Dufrene et al. (2005); Van Wijk et al. (2000)
THETA	Curvature parameter for photosynthesis	0.882	0.9	Yan et al. (2023); Thornley (2002)
VCMAX25	Saturated rate of carboxylation at 25 ºC (µmol m^{-2} s^{-1})	38.9	80.0	*; **
Water exchange				
GSmax	Maximum stomata conductivity (mmol H_2O m^{-2} s^{-1})	497.3	30.0	*; **
GSmin	Minimum stomata conductivity (mmol H2O m^{-2} s^{-1})	9.1	1.5	*; **
H2OREF_GS	Relative available soil water content at which stomata closure starts	0.3	0.0	*; **
WUECmax	Maximum water use efficiency (mg H_2O g C^{-1})	23.7	16.0	*; **
WUECmin	Minimum water use efficiency (mg H_2O g C^{-1})	4.0	6.0	*; **

Phenology				
DLEAFSHED	Total leaf longevity from emergence (days)	350	3180	*; **
GDDFOLSTART	Temperature sum for foliage activity onset (°C)	282	30	*; **
MFOLopt	Foliage biomass for mature stands under closed canopy condition (kg m^{-2})	0.25	1.2	*; **
NDFLUSH	Time interval necessary to complete flushing of foliage (days)	21	30	*; **
NDMORT	Time interval necessary to complete litterfall (days)	106	2815	*; **
SLAmax	Specific leaf area in the shade (m^2 kg^{-1})	31.0	7.5	Aranda et al. (2004); Bartelink (1996)
SLAmin	Specific leaf area in full light (m^2 kg^{-1})	11.0	3.5	Aranda et al. (2004); Bartelink (1996)
Others				
ALB	Foliage albedo	0.05	0.045	Dufrene et al. (2005); Hember et al. (2010)
EXT	Light extinction factor	0.532	0.453	Molina-Herrera et al. (2015); Raj et al. (2018)
KM20	Maintenance coefficient at reference temperature of 20 ºC	0.90	0.45	*; **
NCFOLopt	Optimum nitrogen concentration of foliage (%)	0.0254	0.015	Mellert and Göttlein (2012); Thom et al. (2024)

*defined from joined automated parametrization of a German (Leinefelde, DE-Lnf), a Danish (Soroe, DK-Sor), and a Czech (Stitna, CZ-Stn) site

**defined from joined automated parametrization of a site in Canada (Campbell River) and one from the Netherlands (Speulderbos)

Table S2: Uncertainty in the tree species contribution of flux footprint predictions dependent on different values of the zero-plane displacement (d). 0.66 * ch = d is the standard equation for estimating the zero-plane displacement according to the canopy height (ch, 28m). In reality the multiplication factor can range between 0.5 and 0.8. The measurement height (zm, 46 m) – d has to be considered in the calculation of the flux footprint predictions. The mean species contributions for dependent on the three different values of d are shown, as well as the mean bias error (MBE), mean absolute error (MAE), and root mean square error (RMSE) for the lower and upper limit of the multiplication factor compared to the standard equation.

d (m)	**zm – d (m)**	**Beech (%)**	**Douglas fir (%)**	**MBE (%)**	**MAE (%)**	**RMSE (%)**
0.5 * ch = 14	32	66.79	33.21	±0.25	1.68	2.05
0.66 * ch = 18.5	27.5	66.54	33.46	-	-	-
0.8 * ch = 22.4	23.6	66.11	33.89	±0.44	1.84	2.16

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