Biogeosciences

Supplement of

Spatializing Net Ecosystem Exchange in the Brazilian Amazon biome using the JULES model and vegetation properties

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S.1 Model description

5   To calculate GPP and Respiration, JULES uses several equations based on the limitation factor of three potential photosynthesis rates (Collatz et al., 1991, 1992): Light limitation rate (W_l); Rubisco limited rate (W_c); and Transport of photosynthetic products for C3 and PEP Carboxylase limitation for C4 plants (W_e). One important aspect of calculating W_e and W_c is the dependence on the maximum rate of carboxylation of Rubisco (V_{cmax}) at 25 °C. To calculate V_{cmax} for any temperature, an optimal temperature range is required for each plant functional type (Tupp and Tlow), as described by Clark

10   et al. (2011) (Equation S1):

$$V_{cmax} = \frac{V_{cmax\,25}ft\,(Tc)}{[1+e^{0.3(Tc-Tupp)}][1+e^{0.3(Tlow-Tc)}]}$$ (S1)

where Tc is the canopy (leaf) temperature in Celsius degrees and *ft* is the standard Q_{10} temperature dependence (Equation S2):

$$ft(Tc) = Q_{10,leaf}^{0.1(Tc-25)}$$ (S2)

15   where $Q_{10,\,leaf}$ is 2.0.

        JULES calculates V_{cmax} in 25 °C based on leaf nitrogen content (kg N kg C^{-1}) in each canopy layer (i) (Equation S3):

$$V_{cmax,25,i} = n_{eff}N_{10}e^{-kn(i-1)/10}$$ (S3)

being, kn the extinction coefficient (kn = 0.78, based on Mercado et al., 2007); N_{10} is the top leaf nitrogen content (kg N kg C^{-1}) considering a 10-layer canopy and n_{eff} linearly relates to the concentration of N in leaves to $V_{cmax,\,25}$.

20   Considering the V_{cmax} JULES can calculate the three potentially-limiting rates:

1-Rubisco-limited rate (W_c) (Equation S4)

$$Wc = \begin{cases} V_{c\,max}\left(\frac{c_i-\Gamma}{c_i+K_c\left(1+\frac{O_a}{K_0}\right)}\right), & for\ C3\ plants, \\ V_{cmax}, & for\ C4\ plants . \end{cases}$$ (S4)

where V_{cmax} (mol CO_2 m^{-2} s^{-1}) is the maximum rate carboxylation of Rubisco, ci is the leaf internal carbon dioxide partial pressure (Pa), Γ is the CO_2 compensation point in the absence of mitochondrial respiration (Pa), Oa is the partial pressure of atmospheric oxygen, and K_c and K_o are the Michaelis-Menten parameters for CO_2 and O_2, respectively.

2- Light-limited rate (W_l) (Equation S5)

$$W_l = \begin{cases} \alpha(1-\omega)I_{PAR}\left(\frac{c_i-\Gamma}{c_i+2\Gamma}\right), & for\ C3\ plants, \\ \alpha(1-\omega)I_{PAR}, & for\ C4\ plants. \end{cases} \tag{S5}$$

where ω is the leaf scattering coefficient for PAR, I_{PAR} is the incident photosynthetically active radiation (PAR, mol m^{-2} s^{-1}), and α is the quantum efficiency for photosynthesis (mol CO_2 mol^{-1} PAR).

3- Rate of transport of photosynthetic products (in the case of C$_3$ plants) and PEPCarboxylase limitation (in the case of C$_4$ plants) (W_e) (Equation S6):

$$We = \begin{cases} 0.5 \cdot V_{cmax}, & for\ C3\ plants, \\ 2 \cdot 10^4 \cdot V_{cmax}\frac{c_i}{P*}, & for\ C4\ plants. \end{cases} \tag{S6}$$

where P* is the surface air pressure.

The three potentially-limiting rates are essential to calculating the rate of gross photosynthesis (W) being the smoothed minimum of the three limited rates previously calculated (Equation S7):

$$\begin{cases} \beta_1 W_p^2 - W_p(W_c + W_l) + W_c W_l = 0, \\ \beta_2 W^2 - W(W_p + W_e) + W_p W_e = 0. \end{cases} \tag{S7}$$

where β1 and β2 are co-limitation coefficients (0.83 and 0.9, respectively) and Wp is the smoothed minimum of W$_c$ and W$_l$. The smaller root of each quadratic is selected.

The first step in calculating respiration is to define leaf dark respiration (Rd). Rd is based on a proportion of V$_{cmax.}$(Equation S8)

$$R_d = f_d V_{cmax} \tag{S8}$$

45   being f_d as the dark respiration coefficient.

After defining the leaf dark respiration, JULES can estimate the leaf photosynthesis (Al). Al estimation is based on the difference between gross photosynthesis rate and Rd with a soil moisture stress factor based on Cox et al. 1998 (β) (Equation S9). With the stress factor is possible to represent how the photosynthesis rate falls due to the hydric stress (Equation S10):

$$Al = (W - Rd)\beta \tag{S9}$$

$$\beta = \begin{cases} 1 \, for \Theta > \Theta_c, \\ \frac{\Theta - \Theta_w}{\Theta_c - \Theta_w} \, for \Theta_w < \Theta \leq \Theta_c, \\ 0 \, for \Theta \leq \Theta_w. \end{cases} \tag{S10}$$

being, Θ the actual soil moisture; Θ_c is the soil moisture at the field capacity; Θ_w is the soil moisture at the wilting point.

Leaf photosynthesis is also important to define the stomatal conductance (gs). The estimate is based on the approach of Jacobs (1984), which identified that the difference between internal and external CO_2 concentration at the leaf level can explain the stomatal opening and closure (Equation S11):

$$Al = \frac{gs(C_s - C_i)}{1.6} \tag{S11}$$

where C_s is the leaf surface CO_2 concentration and C_i is the leaf internal CO_2 concentration.

The leaf CO_2 concentration on the surface or internal is defined based on the leaf humidity deficit estimated by the vapor deficit in the leaf surface (D) and in two parameters related to specific plant function types (f_0 and D$crit$) (Equation S12):

$$\frac{C_i - \Gamma}{C_s - \Gamma} = f_0 \left(1 - \frac{D}{Dcrit}\right) \tag{S12}$$

60   To calculate the total plant respiration, JULES considers the sum of two procedures: Growth and maintenance respiration (Rpm and Rpg, respectively, Equations S13 and S14)

$$R_{pm} = 0.012 \cdot R_d \left(\beta + \frac{N_r + N_s}{N_l}\right) \tag{S13}$$

3

and

$$R_{pg} = r_g(GPP - R_{pm}) \tag{S14}$$

where N_l, N_s, and N_r are the nitrogen contents of leaf, stem, and root, respectively, as described by Clark et al. (2011). R_g is the growth respiration coefficient set for 0.25 for all plant functional types (Clark et al., 2011, and Harper et al., 2016). GPP is based on the integration of Al, taking into account every leaf level adopted by Harper et al. (2016) in each used multi-layer canopy with sunlit and shaded leaves in each layer.

To calculate the nitrogen contents of leaves, stems, and roots, leaf area index (LAI) and canopy height are important elements in the estimation, as provided in equations S15, S16, and S17:

$$N_l = n_m \sigma_l L \tag{S15}$$

$$N_s = \mu_{sl} n_m S \tag{S16}$$

$$N_r = \mu_{rl} n_m R \tag{S17}$$

where n_m is the mean leaf nitrogen concentration (kg N (kg C)$^{-1}$), R and S are the quantity of carbon present in the root and respiring stem, L is the canopy leaf area index, and σl (kg C m^{-2} per unit of LAI) is the specific leaf density. The nitrogen contents of roots and stems are assumed to be fixed (functional type dependent) multiples, μ_{rl} and μ_{sl}, of the mean leaf nitrogen concentration: $\mu_{rl} = 1.0$ for all PFTs, $\mu_{sl} = 0.1$ for woody plants (trees and shrubs), and $\mu_{sl} = 1.0$ for grasses. To calculate the respiring stemwood, the pipe model of Shinozaki et al (1964) was utilized, taking into account canopy height, LAI (Equation S18):

$$S = n_{sl} h L \tag{S18}$$

Where n_{sl} is a constant of proportionality from Friends et al (1993), and h is the canopy height.

JULES calculates the net ecosystem exchange (NEE) as the difference between GPP and total ecosystem respiration (plant and soil respiration, R_{eco}, Equation S19):

$$NEE = R_{eco} - \text{GPP} \tag{S19}$$
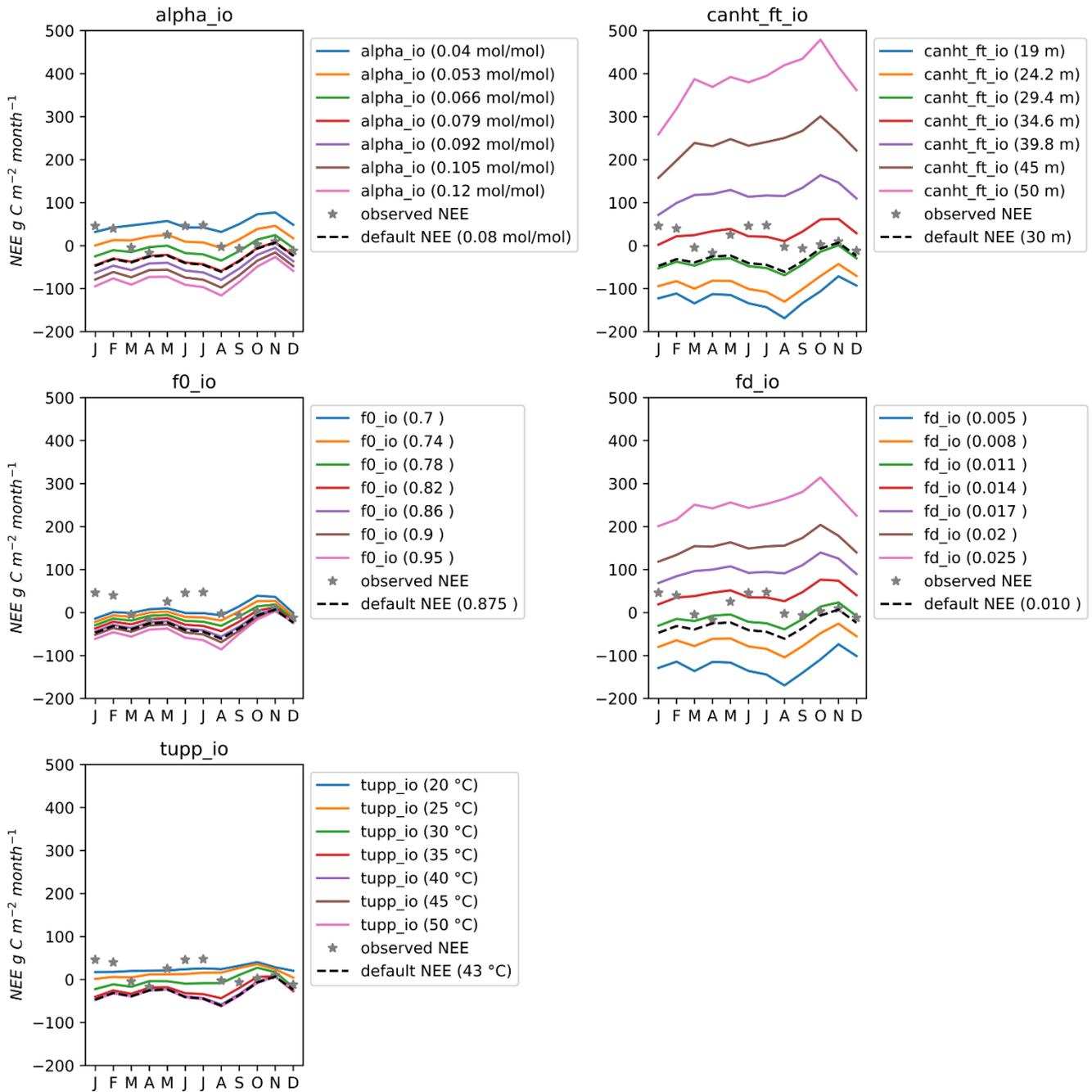
90   **S.2. Sensitivity analysis**

Table S1: JULES parameters selected for sensitivity analysis in the Amazon region based on Li et al. (2016) for broadleaf tree forest. Maximum and minimum values for each parameter were based on the literature

Parameters	Description	minimum value	maximum value
alnir	Leaf reflection coefficient for NIR.	0.225	0.675
alpar	Leaf reflection coefficient for VIS (photosynthetically active radiation, PAR).	0.05	0.15
alpha	Quantum efficiency (mol mol^{-1}).	0.04	0.12
canht_ft	Canopy height (m).	19	50
catch0	Minimum canopy water capacity (kg m^{-2}).	0.25	0.75
dcatch_dlai	Rate of change of canopy water capacity with LAI (kg m^{-2}).	0	0.2
dgl_dt	Rate of change of leaf turnover rate with temperature (K^{-1}).	4.5	13.5
dqcrit	Critical humidity deficit (kg kg^{-1}).	0.045	0.135
dz0v_dh	Rate of change of vegetation roughness length for momentum with height.	0.01	0.15
f0	Values of the maximum ratio of internal to external CO$_2$.	0.7	0.95

Fd	Scale factor for dark respiration.	0.005	0.025
g_leaf_0	Minimum turnover rate for leaves.	0.125	0.375
glmin	Minimum leaf conductance for H2O (mmol $m^{-2}s^{-1}$).	5.00E-07	1.50E-06
kext	Light extinction coefficient- used with Beer's Law for light absorption through tile canopies.	0.25	0.75
kpar	PAR Extinction coefficient (m^2m^{-2}).	0.25	0.75
nl0	Top leaf nitrogen concentration (kg N kg C^{-1}).	0.023	0.069
r_grow	Growth respiration fraction.	0.125	0.375
rootd_ft	Root depth (m).	0.5	6
tleaf_of	Temperature below which leaves are dropped (K).	273.15	283.15
tlow	Lower temperature threshold for photosynthesis (°C).	-5	15
tupp	Upper temperature threshold for photosynthesis (°C).	20	50

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Table S2: Relevance level of JULES parameters in the ATTO tower representing the Brazilian Amazon biome. The most sensitive parameters, highlighted in bold, were chosen based on the shared relevance in NEE simulations.

parameter	MAD (g C m^{-2} day^{-1})	parameter	var(%)
canht_ft_io	**16.5781**	**canht_ft**	**193.38**
fd	**12.3263**	**fd**	**141.81**
alpha	**4.1886**	**alpha**	**45.06**
tupp	**2.0199**	**f0**	**15.93**
f0	**1.6988**	**tupp**	**13.24**
dqcrit	0.8584	dqcrit	11.61
r_grow	0.7734	r_grow	5.79
dz0 max	0.4571	dz0v_dh	5.00
root	0.3521	root	4.66
tlow	0.1391	tlow	1.90
alpar	0.0896	dcatch	1.00
dcatch	0.0788	alpar	0.88
catch0	0.0238	catch0	0.32
kext	0.0046	kext	0.08
glmin	0.0007	glmin	0.02
alnir	0.0000	alnir	0.00
dgl_dt	0.0000	dgl_dt	0.00
kpar	0.0000	kpar	0.00
n10	0.0000	n10	0.00
tleaf	0.0000	tleaf	0.00
gleaf	0.0000	g_leaf	0.00

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Figure S1: Sensitivity analysis of main parameters of JULES for NEE variable in the ATTO tower representing the Brazilian Amazon biome during the year 2018.
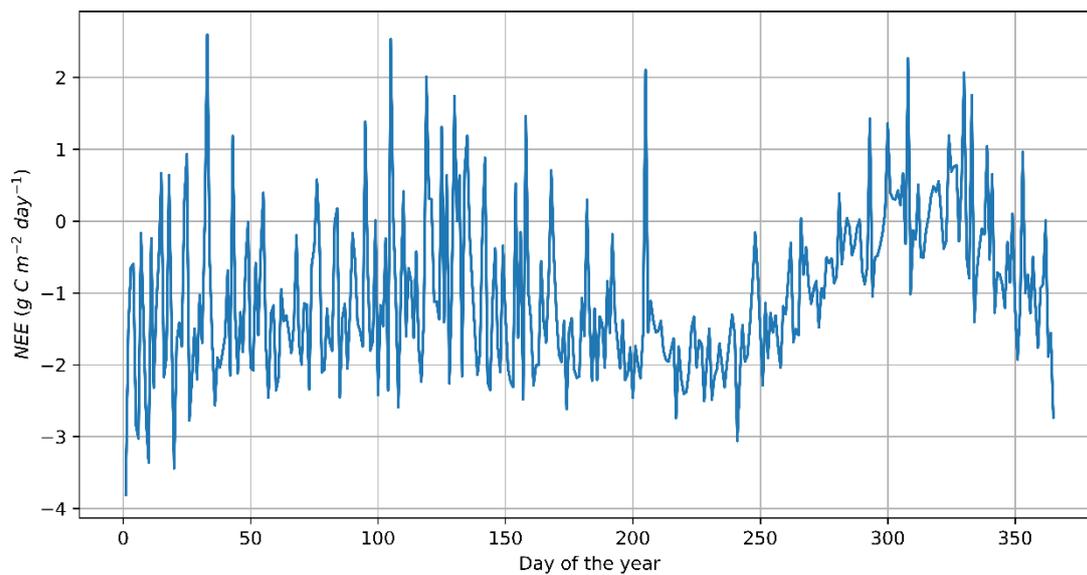
Figure S2: Daily NEE simulated by JULES in the ATTO tower based on Harper et al. (2016) parameters during the year 2018

S.3 Spatialization of JULES parameters

S.3.1. Mapbiomas database adaptation for JULES

Table S3: Mapbiomas classes of vegetation and the respective land functional type from JULES applied to spatialize the Brazilian Amazon biome and land functional type (PFT) available in the JULES model.

Mapbiomas	JULES- PFT	Descrption
Forest Formation	BET-TR	Broadleaf Evergreen trees - tropical
Savannah Formation	ESH	Evergreen shrubs
Mangrove	BET-TR	Broadleaf Evergreen trees - tropical
Floodable Forest	BET-TR	Broadleaf Evergreen trees - tropical
Wooded Sandbank Vegetation	ESH	Evergreen shrubs
Grassland-Savannah	ESH	Evergreen shrubs
Hypersaline Tidal Flat	ESH	Evergreen shrubs
Herbaceous Sandbank Vegetation	ESH	Evergreen shrubs
Pasture	C4	C4 grass
Soybean	C3	C3 grass and crops
Sugarcane	C4	C4 grass
Rice	C3	C3 grass and crops
Cooton	C3	C3 grass and crops
Perennial crop	ESH	Evergreen shrubs
Forest Plantation	BDT	Broadleaf Deciduous Trees
Beaches, dunes, and sand spots	Bare soil	Bare soil
Urban Area	Urban	Urban
Mining	Bare soil	Bare soil
River, Lake, and Ocean	Water	Water
Aquaculture	Water	Water
Not observed	Bare soil	Bare soil
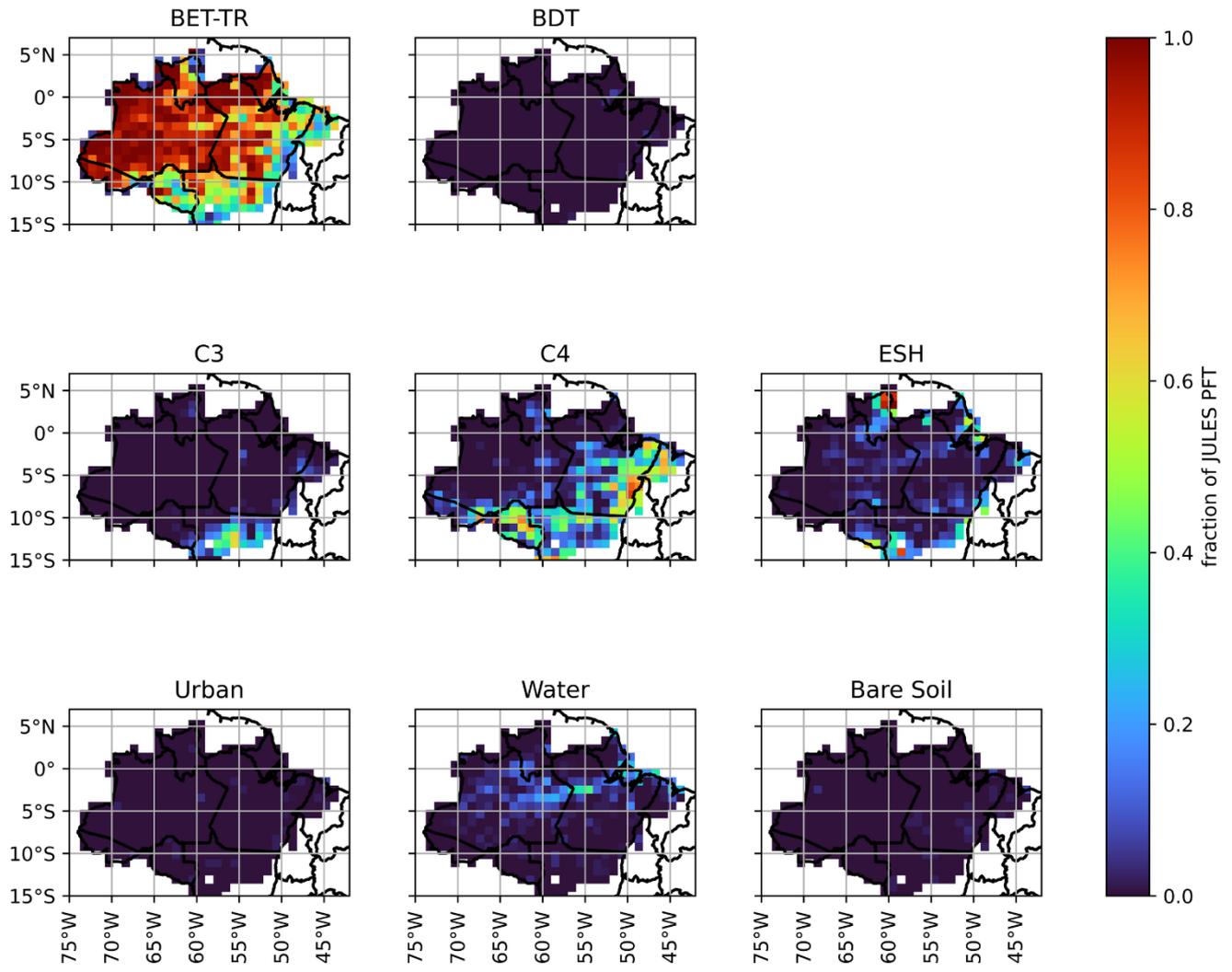
Figure S3: Distribution of each JULES plant and non-plant functional type in the S3.2.1 utilized for spatializing the carbon flux simulations.

S.3.2. Tupp, upper temperature threshold for photosynthesis

Two linear regression models were tested for the parameter tupp, having the canopy height of the LAI as predictors. Tupp showed a directly proportional relationship with LAI and an inversely proportional relationship with the canopy height (Figure S5). Physically, it makes sense to have an inverse relationship between tupp and canopy height, since low-canopy plants like

135 C4 typically have higher temperature thresholds for photosynthesis. On the other hand, a positive relationship between tupp and LAI is not physically consistent, since forest areas with higher LAI are expected to have lower temperature thresholds for photosynthesis Li et al. (2016). Considering the arc of deforestation predominantly occupied by C4 grasses, the utilization of canopy height to spatialize tupp resulted in higher values distributed in this zone. Obviously, since this is an inverse linear relationship, tupp regression values were limited to 45ºC. Otherwise, the regression model would deliver unrealistically high

140 values. The 45 °C limit was based on Harper et al. (2016), which defined a tupp of 45 °C for C4 grasses based on a field experiment in Tapajos. This is higher than the value used by Osborne et al (2015) for soybean (36 ºC) and near the tupp value for Maize (45 °C). In the forest areas, the parameterization of tupp using canopy height as a predictor results in a range of values from 37 ºC. In regions with high canopy height, such as in K67 and RJA towers (36 m and 35 m), to 42 ºC in the ATTO and K34 towers, with a lower canopy height (30 and 27 m, respectively) but a higher LAI (5,46 and 4,79 m^2 m^{-2}, respectively).
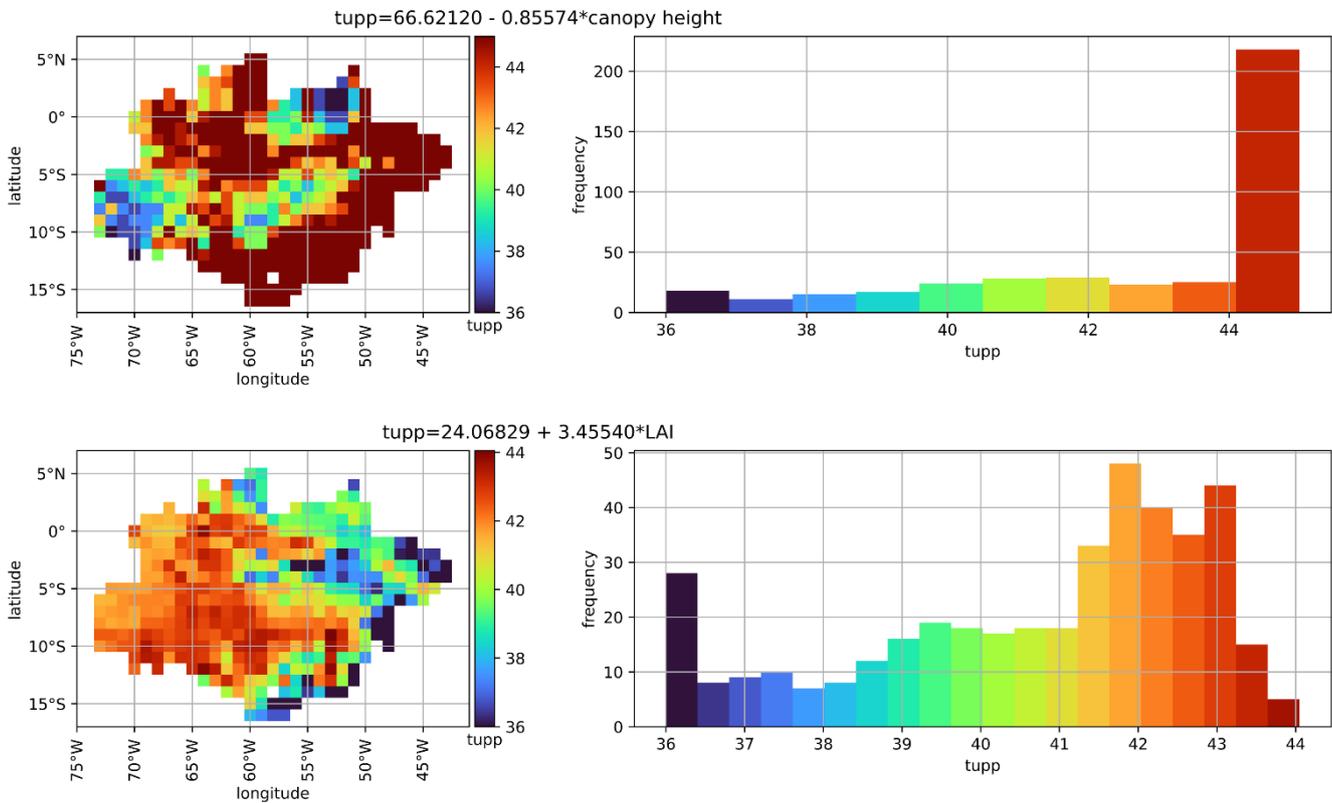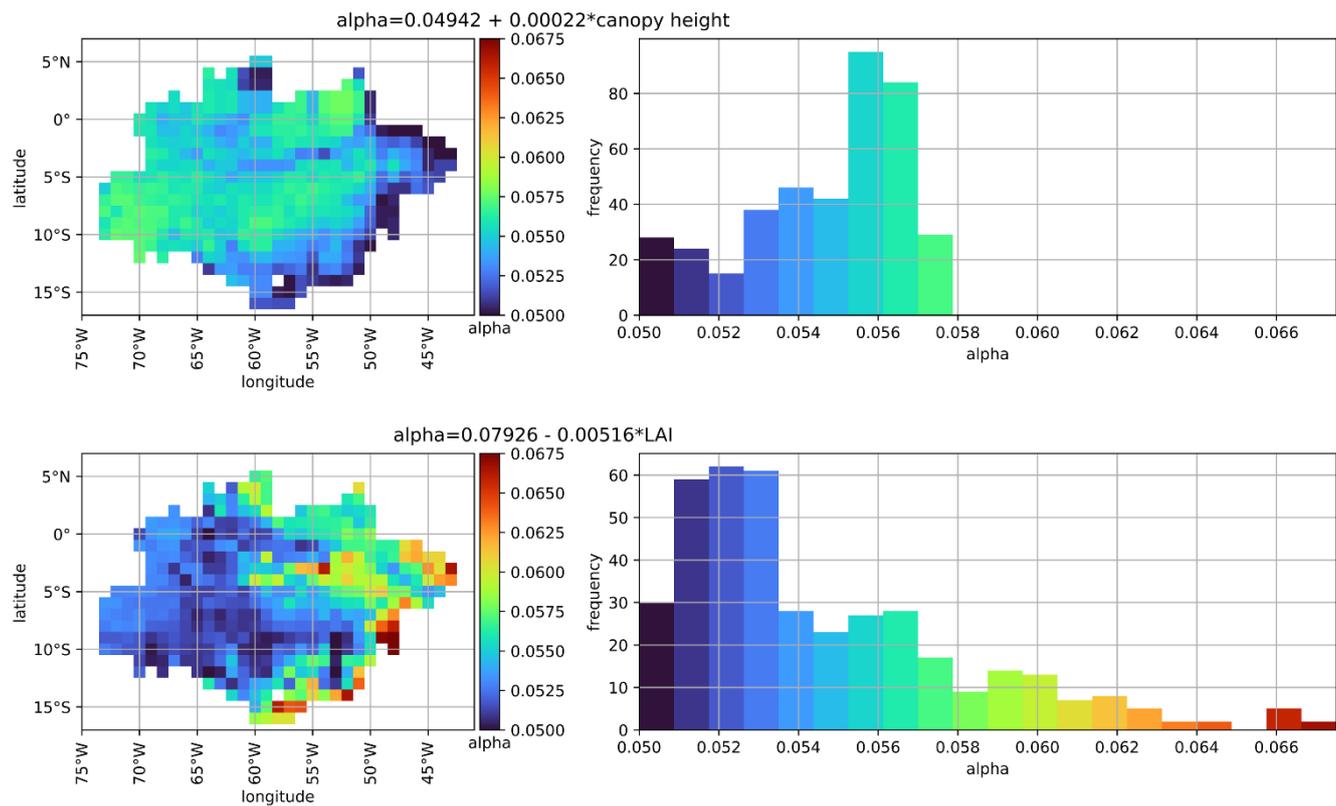

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Figure S4: Tupp spatialized for the Brazilian Amazon biome using two different predictors, canopy height and LAI.
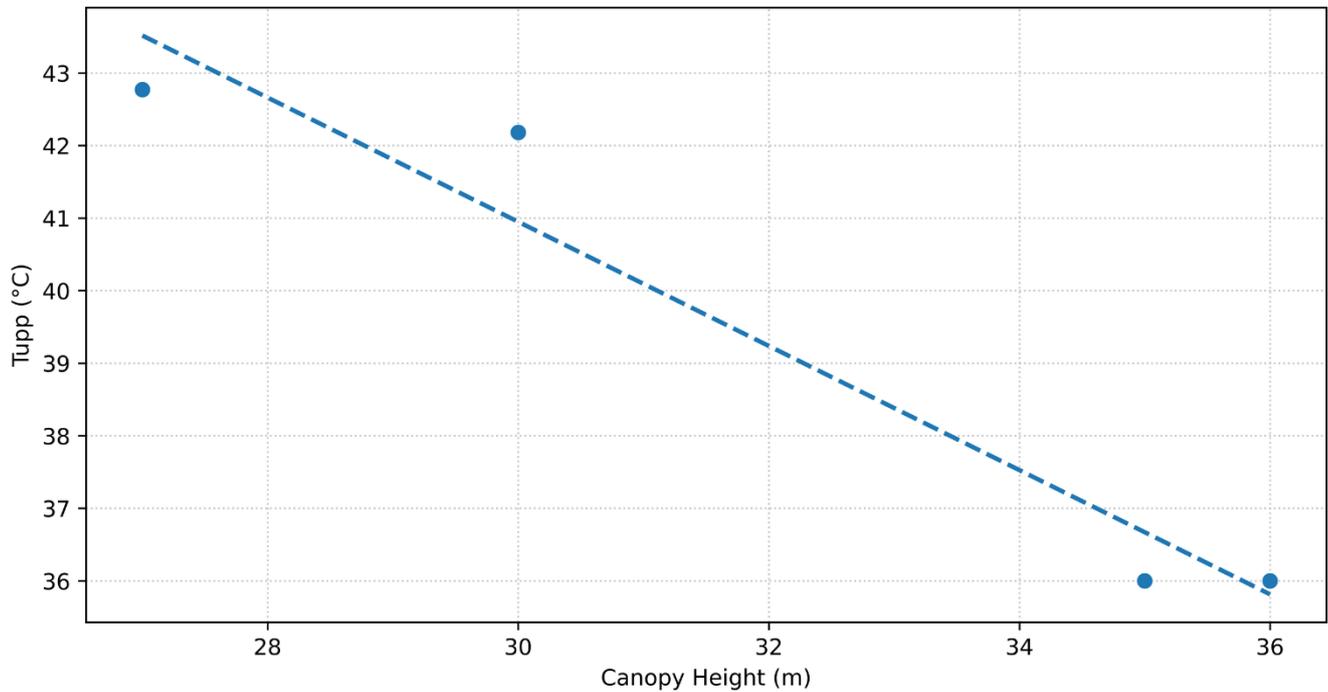
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Figure S5: Relationship between Canopy Height and Tupp (ºC) for different sites of the Brazilian Amazon biome.

S.3.3. alpha, quantum efficiency

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Regarding the parameter alpha, the best alternative for spatialization is to use canopy height (Figure S6), as demonstrated by Harper et al. (2016). Tropical forests are more efficient in converting PAR into carbon when compared to C4 plants (Harper et al., 2016). Using the canopy height as a predictor, the alpha values for forested regions were in the range 0.05 to 0.06 mol[1]

160 mol^{-1}, consistent with Skillman (2008), who evaluated different species of C3 plants.
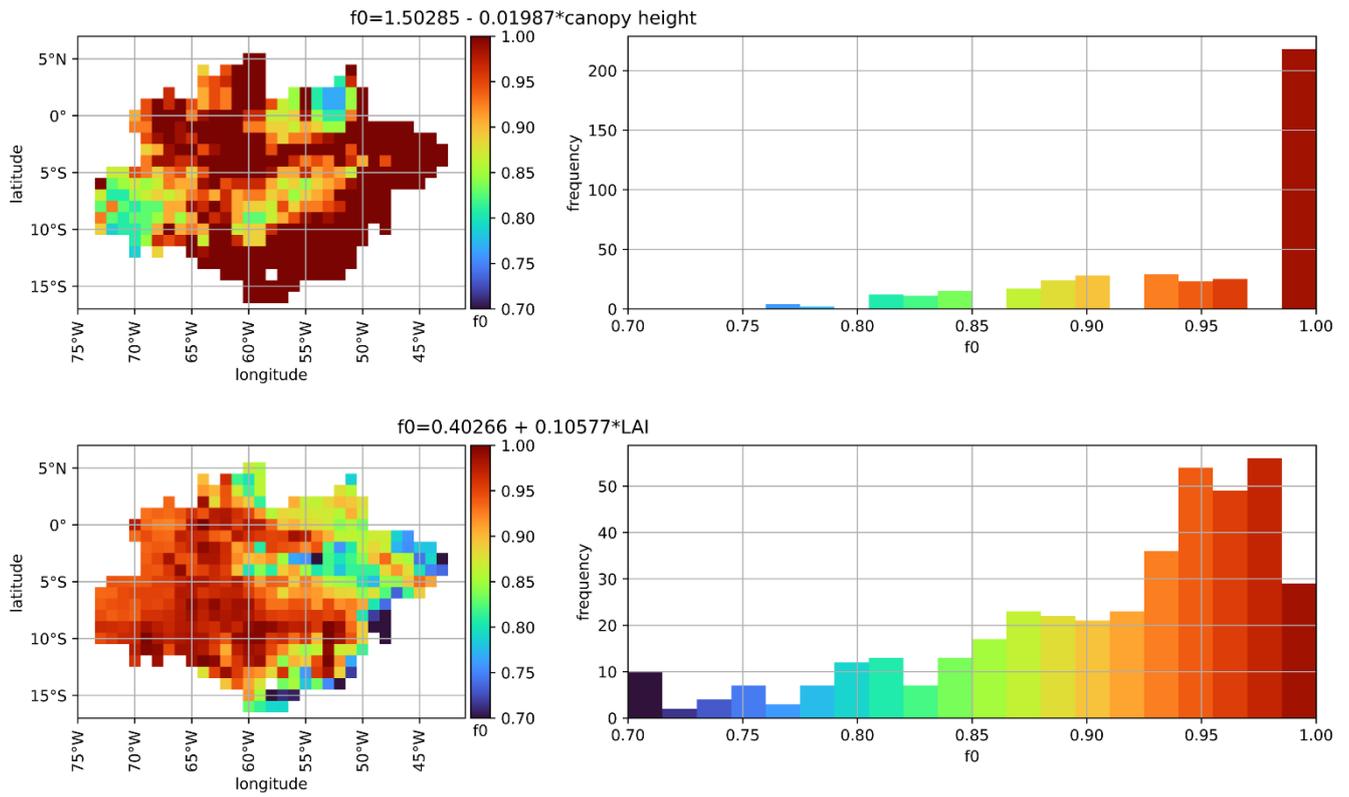
Figure S6: Alpha spatialized for the Brazilian Amazon biome using two different methods, with canopy height and LAI.
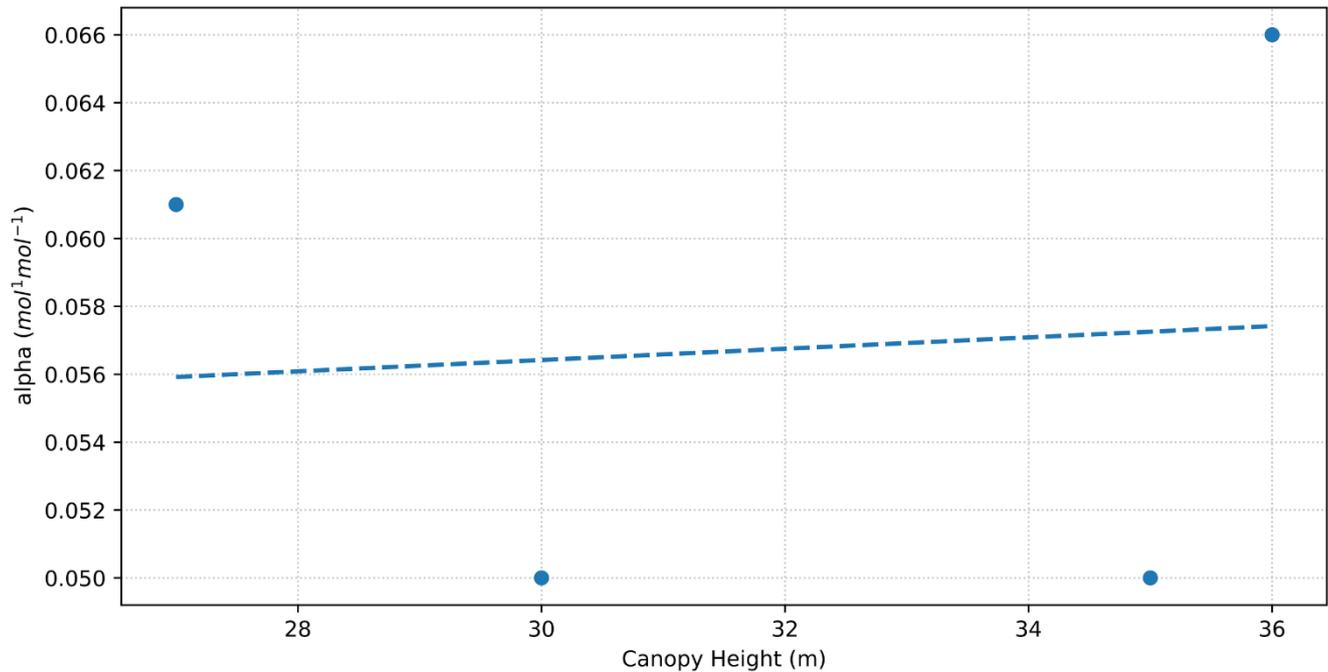
Figure S7: Relationship between Canopy Height (m) and alpha (mol^1 mol^{-1}) for different sites of the Brazilian Amazon biome.

S.3.4. f0, maximum ratio of internal to external CO$_2$

The parameter f0 controls the maximum values of leaf-level stomatal conductance. It is a dimensionless quantity ranging from 0 to 1, being associated with water use efficiency. As such, lower f0 values are expected for plants that are more efficient in water use. Despite canopy height representing better tupp and alpha spatialized, the best alternative for f0 is to use LAI (Figure S8). LAI can represent the expected reduction of this parameter in the arc of deforestation. C4 plants are more efficient in water use, using less water to produce biomass, due to their metabolism. In a condition of high temperature and radiation, C4 plants reduce the Rubisco oxygenase activity and hence the photorespiration (Lambers et al., 2008). In Harper et al. (2016), f0 showed lower values for C4 plants than for tropical forests (0.8 and 0.875, respectively). The same concept can be applied in the center of the forest, where Santarem and Jaru have species more adaptable to longer dry seasons than the ATTO tower and Manaus. Accordingly, the parametrization of f0 based on LAI retrieved lower values in Santarem.

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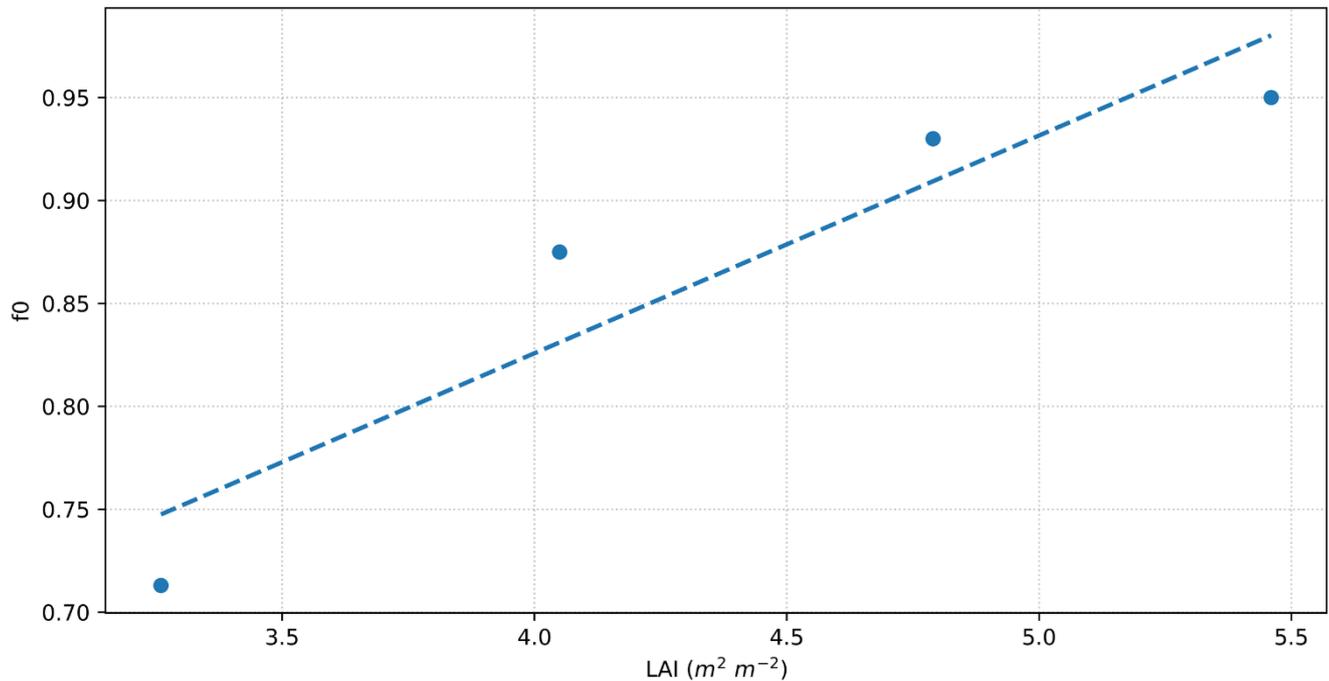**Figure S8: f0 spatialized for the Brazilian Amazon biome using two different methods, with canopy height and LAI.**

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Figure S9: Relationship between LAI and f0 for different sites of the Brazilian Amazon biome.

S.3.5. fd, scale factor for dark respiration

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Similarly to f0, the parameter fd was better represented in the Amazon Basin using LAI (Figure S11). C4 plants, as the tropical pastures widely used in Brazil, such as Marandu (*Urochloa brizantha* cv Marandu), are more efficient in the utilization of water. The high-water efficiency of C4 plants occurs due to the metabolism that increases carbon concentration in the stomata, reducing photorespiration. Thus, the parameter fd should be lower for this type of plant than for forest species. Using

190 LAI to extrapolate fd for the Amazon Basin resulted in values ranging from 0.005 in the arc of deforestation to 0.015 in forested areas (Figure S10). The resulting fd values are relatively small compared to references like: 0.019 for C4 grass (Harper et al., 2016), 0.0096 for maize (Williams et al., 2017), and 0.008 for maize (Leung et al., 2020). However, the same studies proposed reductions in the fd values compared to the default ones, indicating that the calibration of this parameter still need improvements in different PFTs.
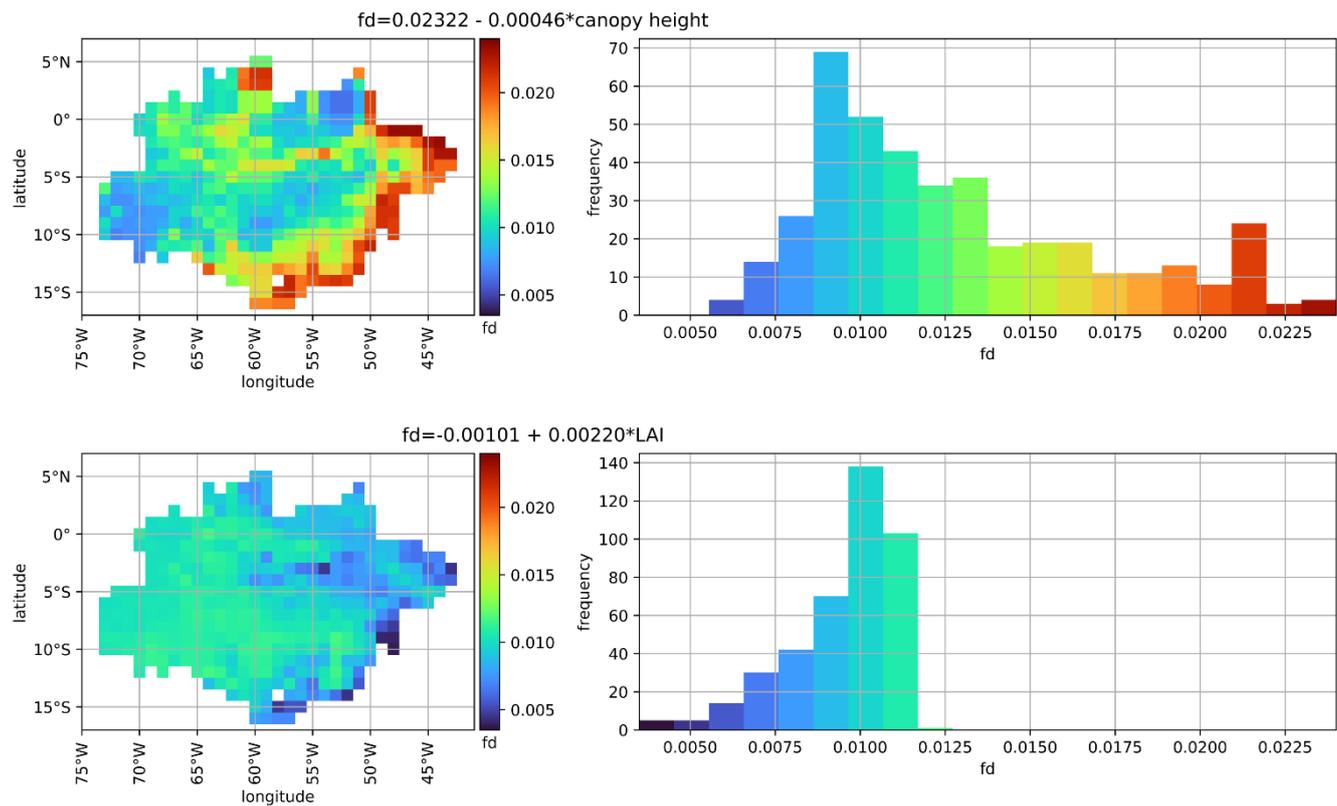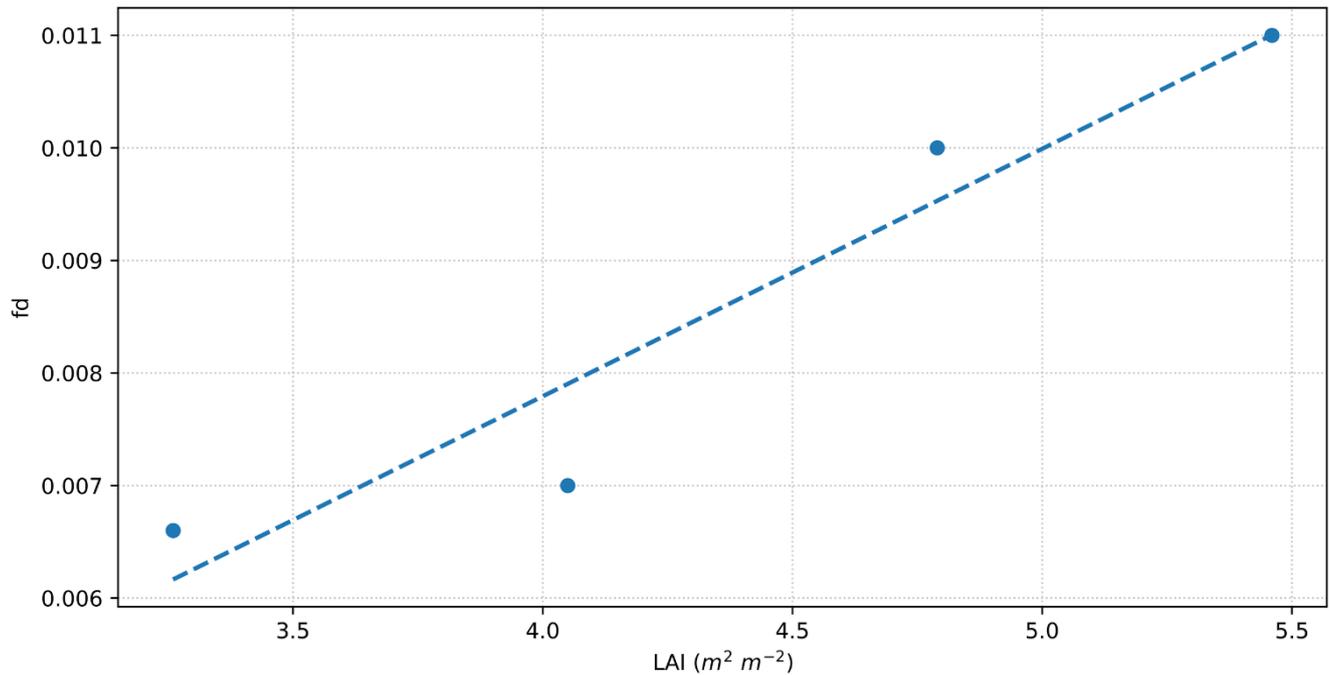
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Figure S10: fd spatialized for the Brazilian Amazon biome using two different methods, with canopy height and LAI.

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**Figure S11: Relationship between LAI and f0 for different sites of the Brazilian Amazon biome.**

S.4. Calibration and evaluation of JULES

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Table S4: Physiological limits for JULES most sensitivies parameters for tropical forests applied for Nelder Mead optimization

Parameter	Physiological limit	unit	Minimum Reference	Maximum Reference
tupp_io	36 - 45	Celsius degree	Clark et al., 2012	Dreyer et al., 2001
alpha_io	0.05 - 0.011	mol CO_2 per mol PAR photons	Sklimmann 2008	Sklimmann 2008
fd_io	0.005 - 0.015	dimensionless	Clark et al., 2011	Harper et al., 2016
f0_io	0.7 - 0.95	dimensionless	Li et al., 2016	Li et al., 2016
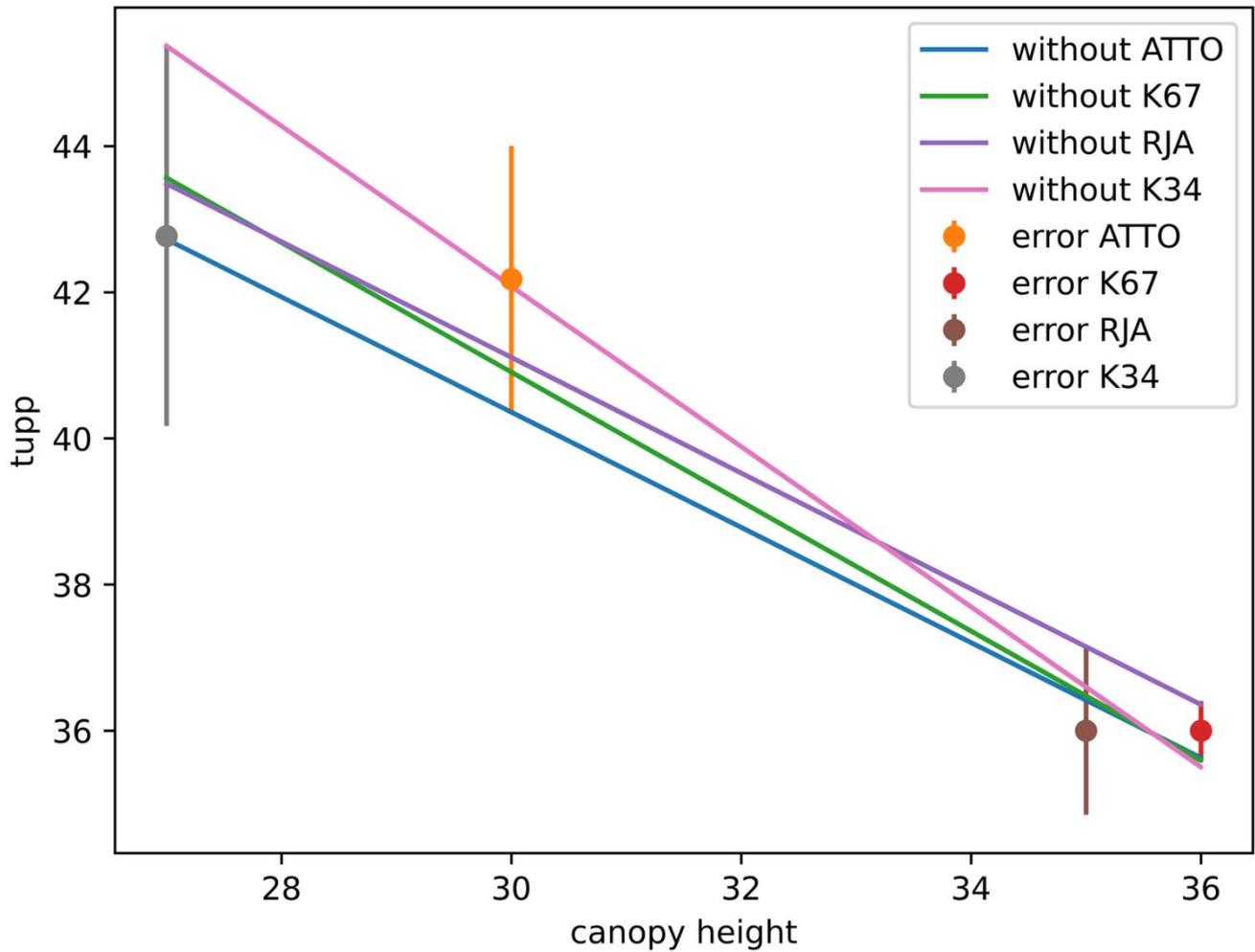
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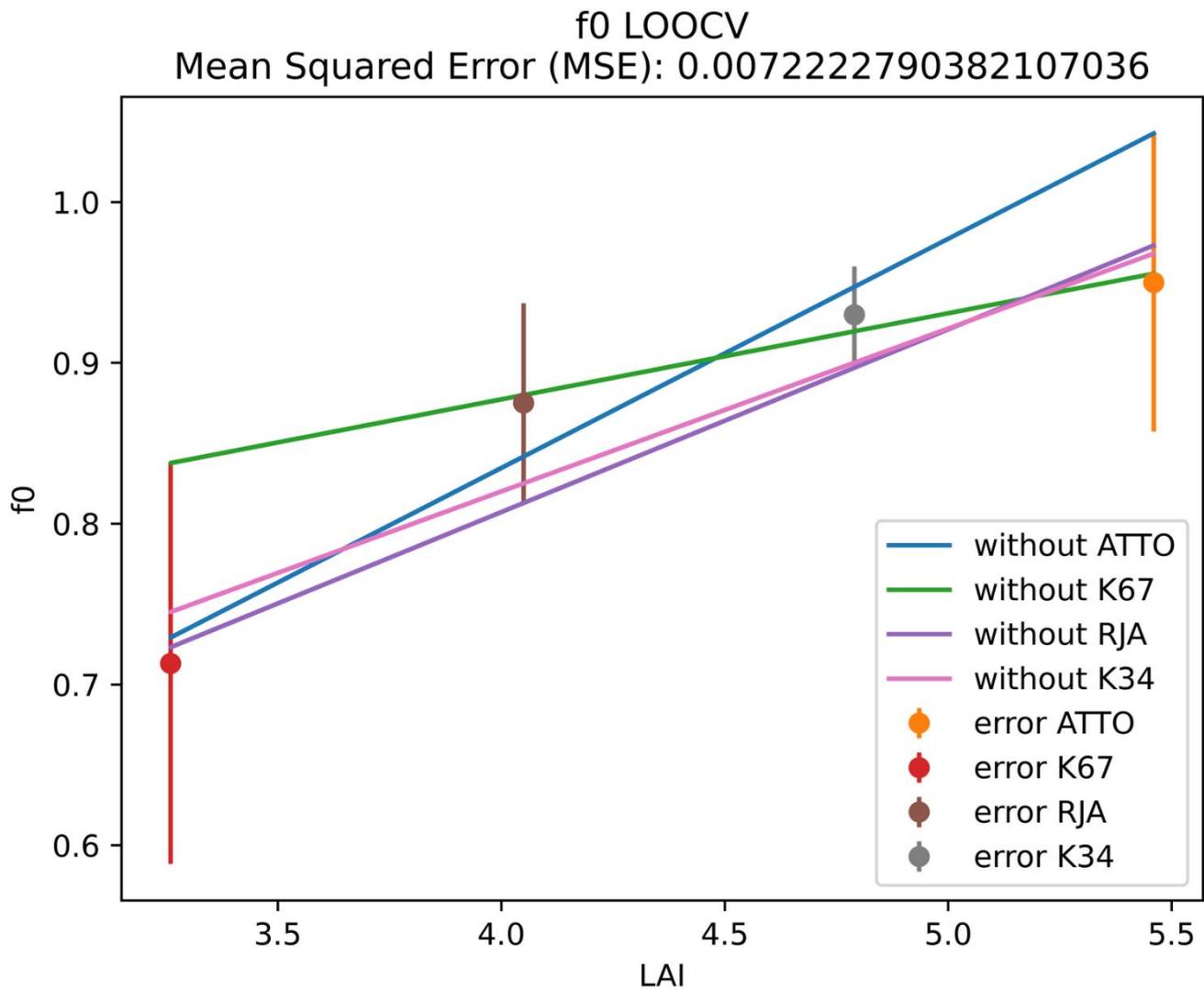**Figure S12: Leave-one-out cross-validation (LOOCV) for Tupp in relation to canopy height for four different towers in the Brazilian Amazon biome.**
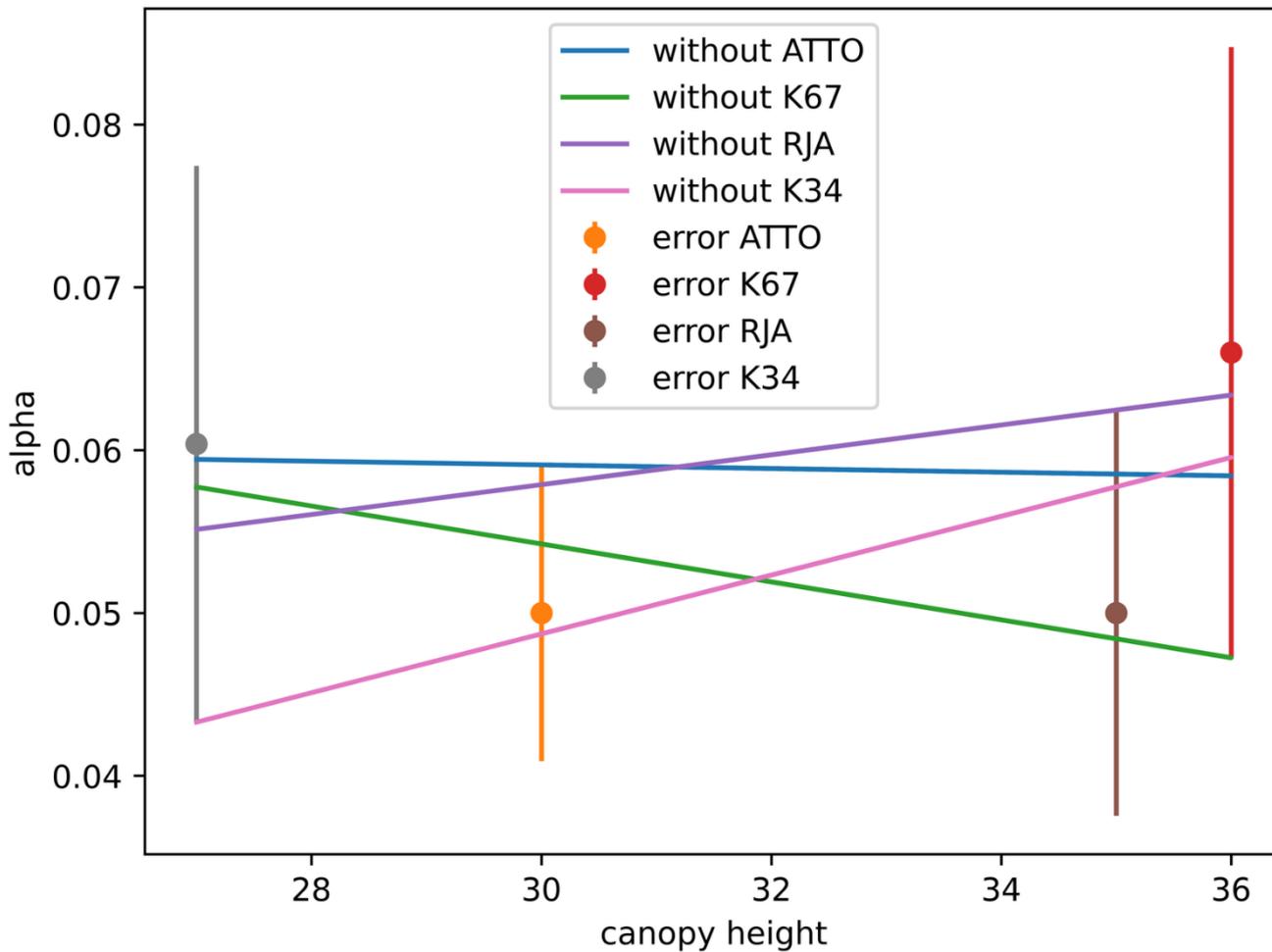
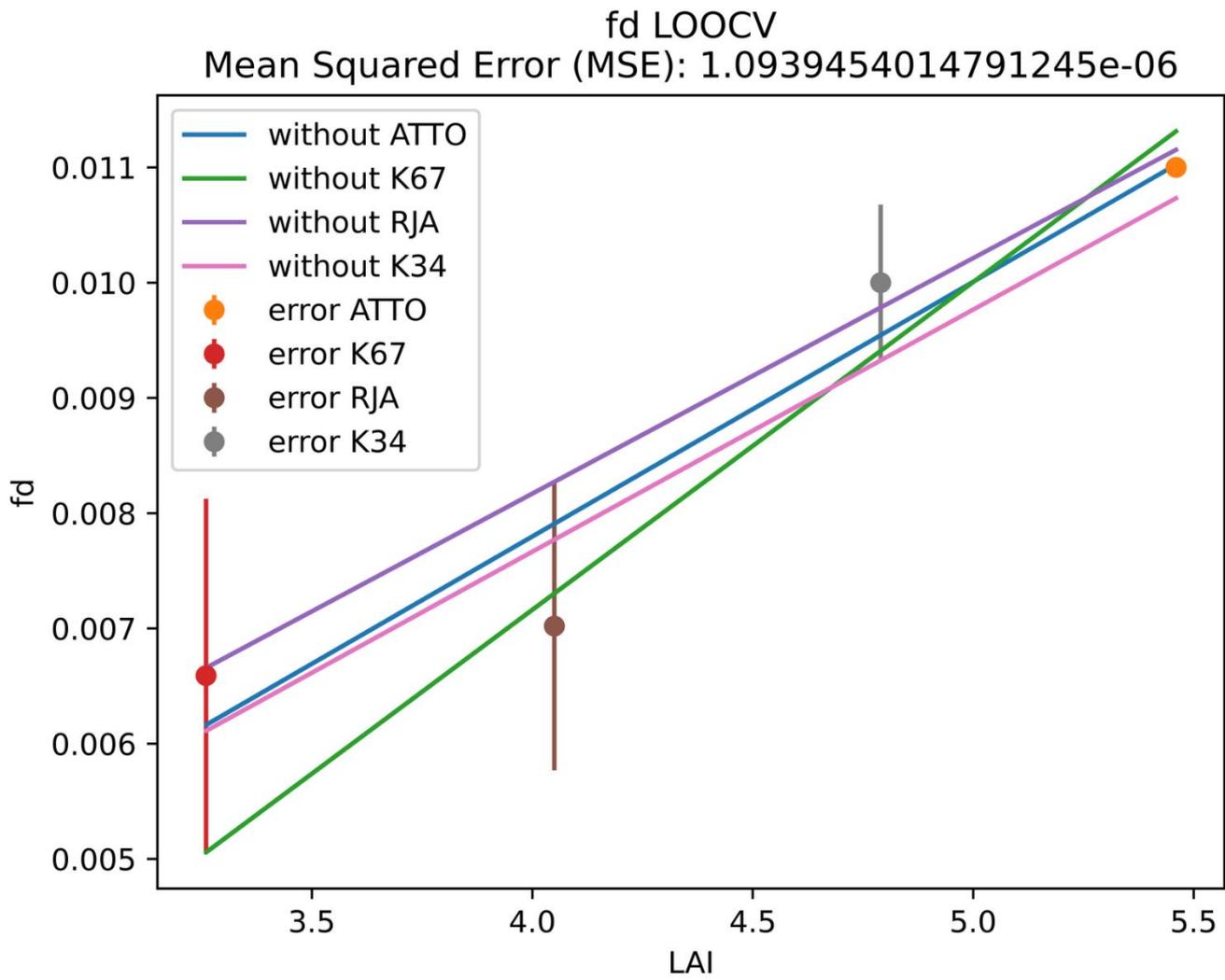**Figure S13: Leave-one-out cross-validation (LOOCV) for alpha in relation to canopy height for four different towers in the Brazilian Amazon biome.**

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Figure S14: Leave-one-out cross-validation for f0 in relation to LAI for four different towers in the Brazilian Amazon biome.
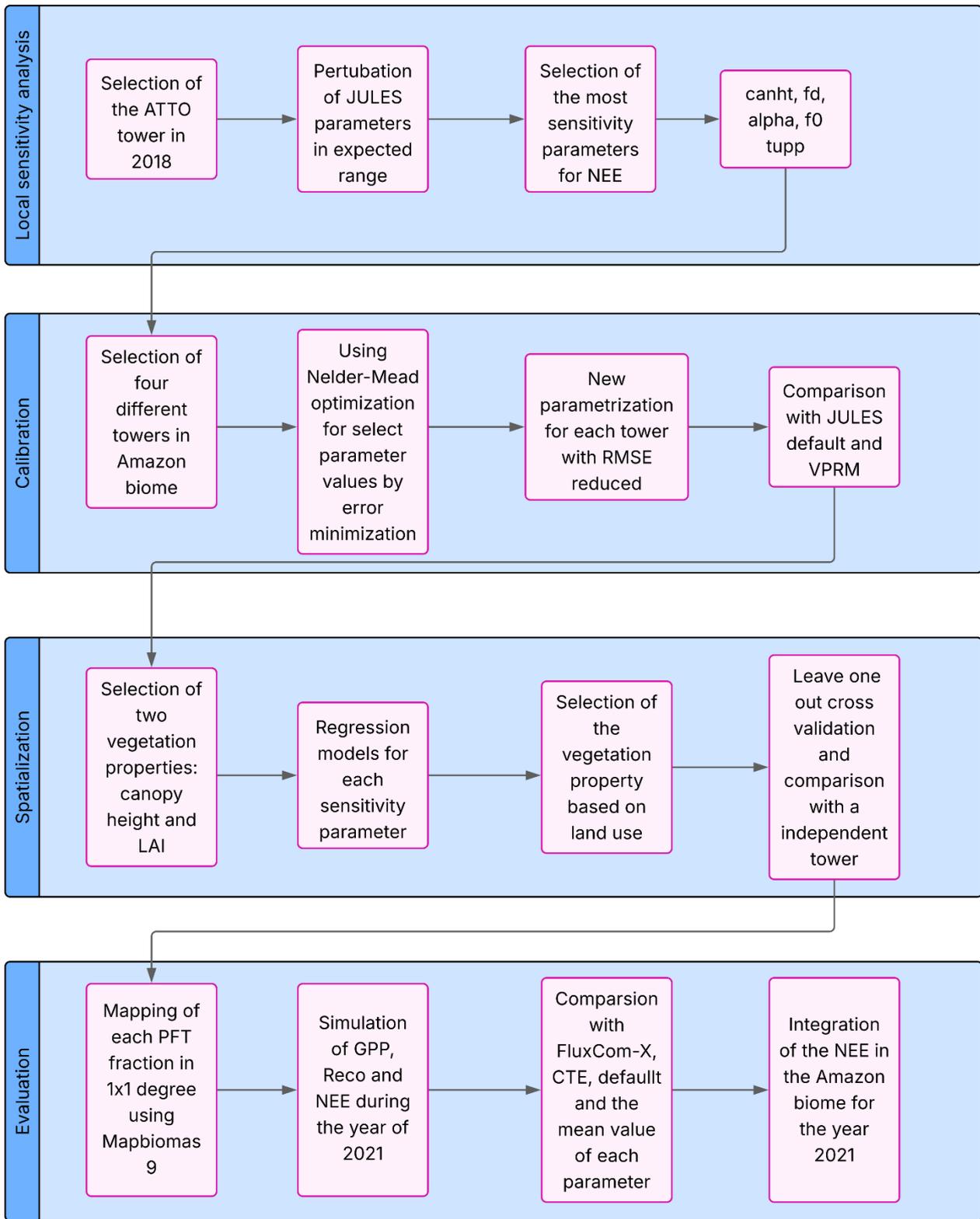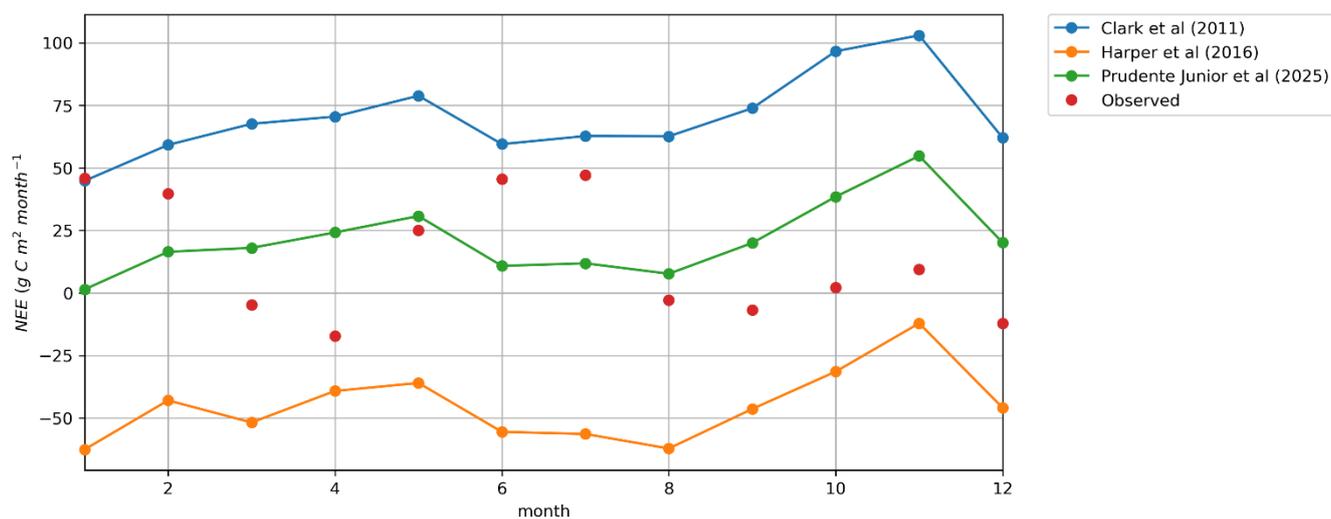
Figure S15: Leave-one-out cross-validation for fd in relation to LAI for four different towers in the Brazilian Amazon
225 **biome.**

Figure S16: Flowchart describing the procedures utilized to spatialize JULES and to obtain the NEE in the Brazilian Amazon biome.

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S.5 Comparison with JULES versions

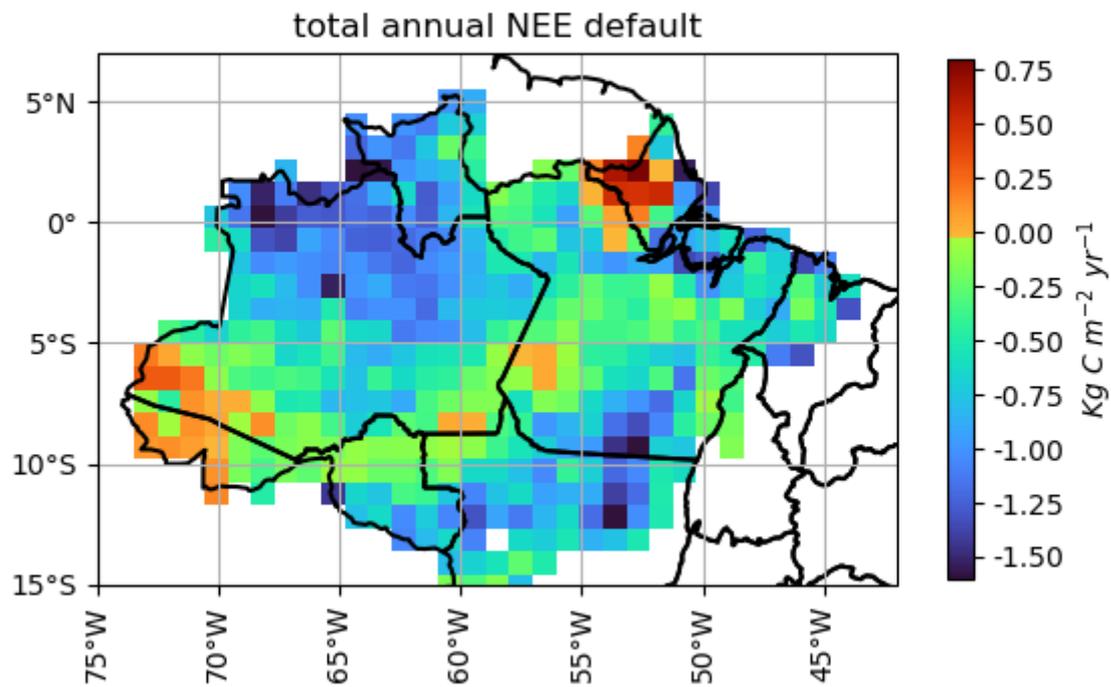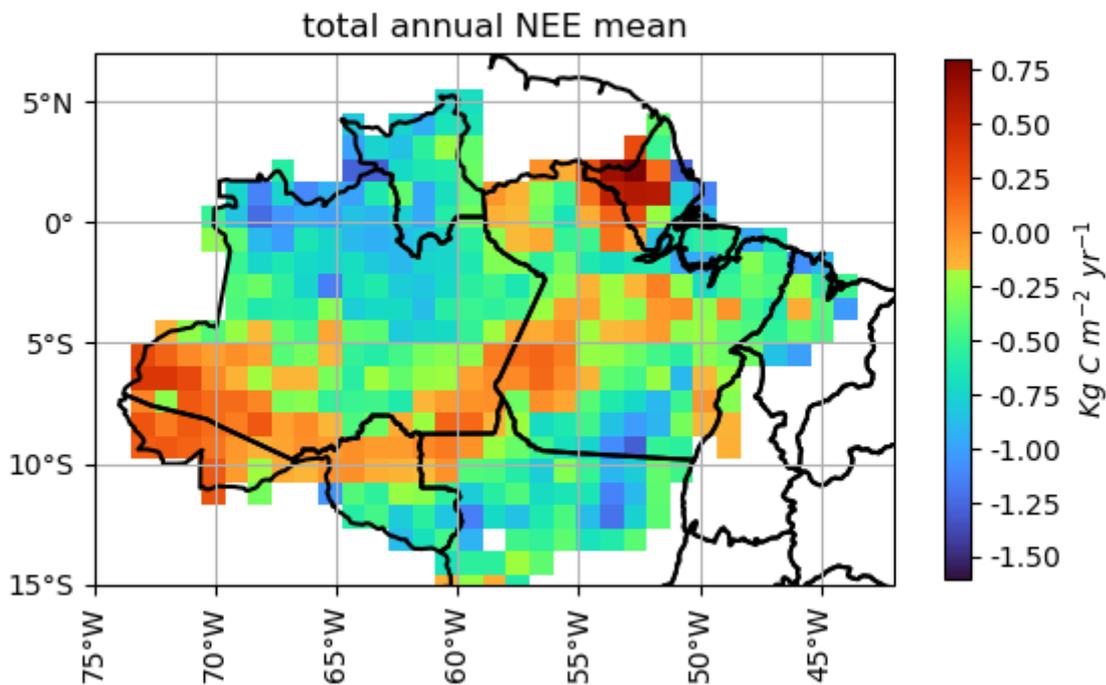235   **Figure S17: Comparison of NEE simulated in different JULES versions in the ATTO tower during the year 2018.**

Figure S18: NEE accumulated in Kg C m⁻² during 2021 in the Brazilian Amazon biome in the default version of JULES (Harper et al., 2016).

Figure S19: NEE accumulated in Kg C m⁻² during 2021 in the Brazilian Amazon biome with the mean value of the JULES parameters optimized.

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