Supplementary material

S.1 Model description

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 et al., (2011) (Equation 1):

$$Vc\,max = \frac{Vcmax{,}25ft(Tc)}{\left[1+e^{0.3(Tc-Tupp)}\right]\left[1+e^{0.3(Tlow-Tc)}\right]} \tag{1}$$

where Tc is the canopy (leaf) temperature in Celsius degrees and *ft* is the standard Q_{10} temperature dependence (Equation 2):

$$ft(Tc) = Q_{10,leaf}^{0.1(Tc-25)} \tag{2}$$

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 3):

$$Vcmax, 25, i = n_{eff} N_{10} e^{-kn(i-1)/10} \tag{3}$$

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.

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

1-Rubisco-limited rate (W_c) (Equation 4)

$$Wc = \begin{Bmatrix} Vcmax\left(\frac{ci-\Gamma}{ci+kc\left(1+\frac{Oa}{ko}\right)}\right) for C3 plants \\ Vc\,max\ for C4 plants \end{Bmatrix} \tag{4}$$

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 Kc and Ko are the Michaelis-Menten parameters for CO_2 and O_2, respectively.

2- Light-limited rate (W_l) (Equation 5)

$$W_l = \begin{Bmatrix} \alpha(1-\omega)Ipar\left(\frac{ci-\Gamma}{ci+2\Gamma}\right) forC3plants \\ \alpha(1-\omega)IparforC4plants \end{Bmatrix} \quad (5)$$

where ω is the leaf scattering coefficient for PAR, *Ipar* 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 6):

$$We = \begin{Bmatrix} 0.5V_{cmax}forC3plants \\ 2x10^4V_{cmax}\frac{ci}{P*}forC4plants \end{Bmatrix} \quad (6)$$

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 7):

$$\begin{Bmatrix} \beta_1 W_p^2 - W_p(W_c + W_l) + W_c W_l = 0 \\ \beta_2 W^2 - W\left(W_p + W_e\right) + W_p W_e = 0 \end{Bmatrix} \quad (7)$$

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 proportional of $V_{cmax.}$(Equation 8)

$$Rd = f_d V_{cmax} \quad (8)$$

being f_d as the dark respiration coefficient.

After defining the leaf dark respiration, JULES can estimate the leaf photosynthesis (*Al*) based on the difference between gross photosynthesis rate and *Rd* and a soil moisture stress factor based on Cox et al., 1998 (β) (Equation 9) in which that can represent how the photosynthesis rate falls due the hydric stress (Equation 10):

$$Al = (W - Rd)\beta \quad (9)$$

$$\beta = \begin{Bmatrix} 1 for \Theta > \Theta_c \\ \frac{\Theta - \Theta_w}{\Theta_c - \Theta_w} for \Theta_w < \Theta \leq \Theta_c \\ 0 for \Theta \leq \Theta_w \end{Bmatrix} \quad (10)$$

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

Leaf photosynthesis is also important to define the stomatal conductance (gs), based on the approach of Jacobs (1984) which identified that the difference between internal and external CO_2 concentration in a leaf level can explain the stomatal open and closure (Equation 11):

$$Al = \frac{gs(C_s - C_i)}{1.6} \quad (11)$$

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 12):

$$\frac{C_i - \Gamma}{C_s - \Gamma} = f_0 \left(1 - \frac{D}{Dcrit}\right) \quad (12)$$

To calculate the total plant respiration, JULES considers the sum of two procedures: Growth and maintenance respiration (Rpm and Rpg, respectively, Equation 13 and 14, respectively)

$$Rpm = 0.012 R_d \left(\beta + \frac{N_r + N_s}{N_l}\right) \quad (13)$$

and

$$R_{pg} = r_g(GPP - R_{pm}) \quad (14)$$

where N_l, N_s and N_r are 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.

The net ecosystem exchange (NEE) is calculated by JULES as the difference between GPP and total ecosystem respiration (plant and soil respiration, $R_{eco,}$ Equation 15):

$$NEE = R_{eco} - \text{GPP} \quad (15)$$

S.2. Sensivitivity analysis

Table S2.1: 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 in 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).	0.05	0.15
alpha	Quantum efficiency (mol/mol).	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).	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 ($mmol/m^2/s$).	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^2/m^2).	0.25	0.75
nl0	Top leaf nitrogen concentration (kg N/kg C).	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

Table S2.2: 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	MDA (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

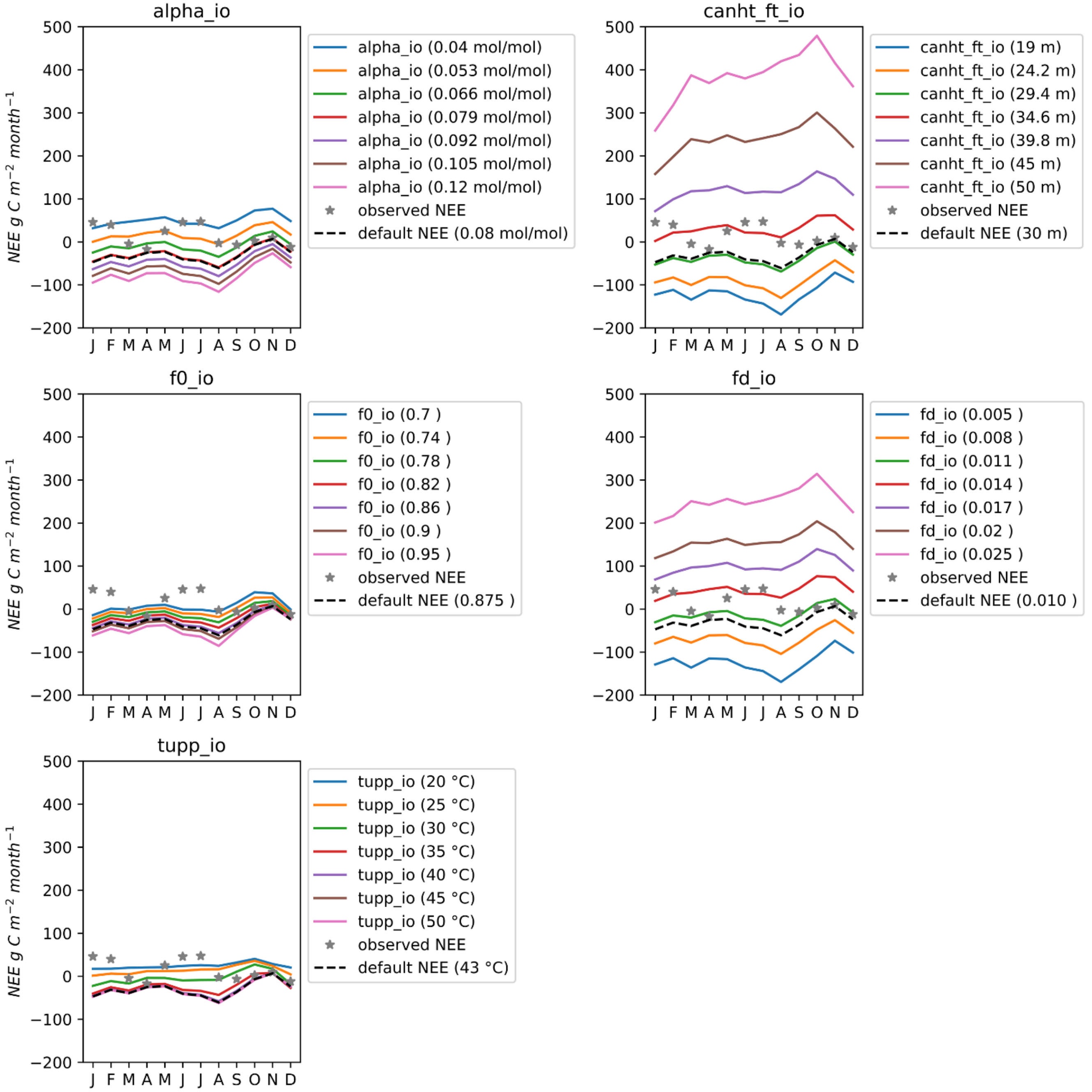
alpha_io
NEE g C m⁻² month⁻¹
alpha_io (0.04 mol/mol)
alpha_io (0.053 mol/mol)
alpha_io (0.066 mol/mol)
alpha_io (0.079 mol/mol)
alpha_io (0.092 mol/mol)
alpha_io (0.105 mol/mol)
alpha_io (0.12 mol/mol)
observed NEE
default NEE (0.08 mol/mol)
canht_ft_io
canht_ft_io (19 m)
canht_ft_io (24.2 m)
canht_ft_io (29.4 m)
canht_ft_io (34.6 m)
canht_ft_io (39.8 m)
canht_ft_io (45 m)
canht_ft_io (50 m)
observed NEE
default NEE (30 m)
f0_io
NEE g C m⁻² month⁻¹
f0_io (0.7)
f0_io (0.74)
f0_io (0.78)
f0_io (0.82)
f0_io (0.86)
f0_io (0.9)
f0_io (0.95)
observed NEE
default NEE (0.875)
fd_io
fd_io (0.005)
fd_io (0.008)
fd_io (0.011)
fd_io (0.014)
fd_io (0.017)
fd_io (0.02)
fd_io (0.025)
observed NEE
default NEE (0.010)
tupp_io
NEE g C m⁻² month⁻¹
tupp_io (20 °C)
tupp_io (25 °C)
tupp_io (30 °C)
tupp_io (35 °C)
tupp_io (40 °C)
tupp_io (45 °C)
tupp_io (50 °C)
observed NEE
default NEE (43 °C)
J F M A M J J A S O N D

Figure S2: Sensitivity analysis of main parameters of JULES for NEE variable in ATTO tower representing the Brazilian Amazon biome during the year of 2018.

S.3 Spatialization of JULES parameters

S.3.1. Mapbiomas database adaptation for JULES

Table S3.1.1: Mapbiomas classes of vegetation and the respective land functional type from JULES applied to spatialize the Brazilian Amazon biome and land functional type (LFT) available in JULES model.

Mapbiomas	JULES- LFT	Descrption
Forest Formation	BET-TR	Broadleaf Evergreen tress - tropical
Savannah Formation	ESH	Evergreen schrubs
Mangrove	BET-TR	Broadleaf Evergreen tress - tropical
Floodable Forest	BET-TR	Broadleaf Evergreen tress - tropical
Wooded Sandbank Vegetation	ESH	Evergreen schrubs
Grassland-Savannah	ESH	Evergreen schrubs
Hypersaline Tidal Flat	ESH	Evergreen schrubs
Herbaceous Sandbank Vegetation	ESH	Evergreen schrubs
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
Perenial crop	ESH	Evergreen schrubs

Forest Plantation	BDT	Broadleaf Decidious Trees
Beaches, dune and sand spot	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

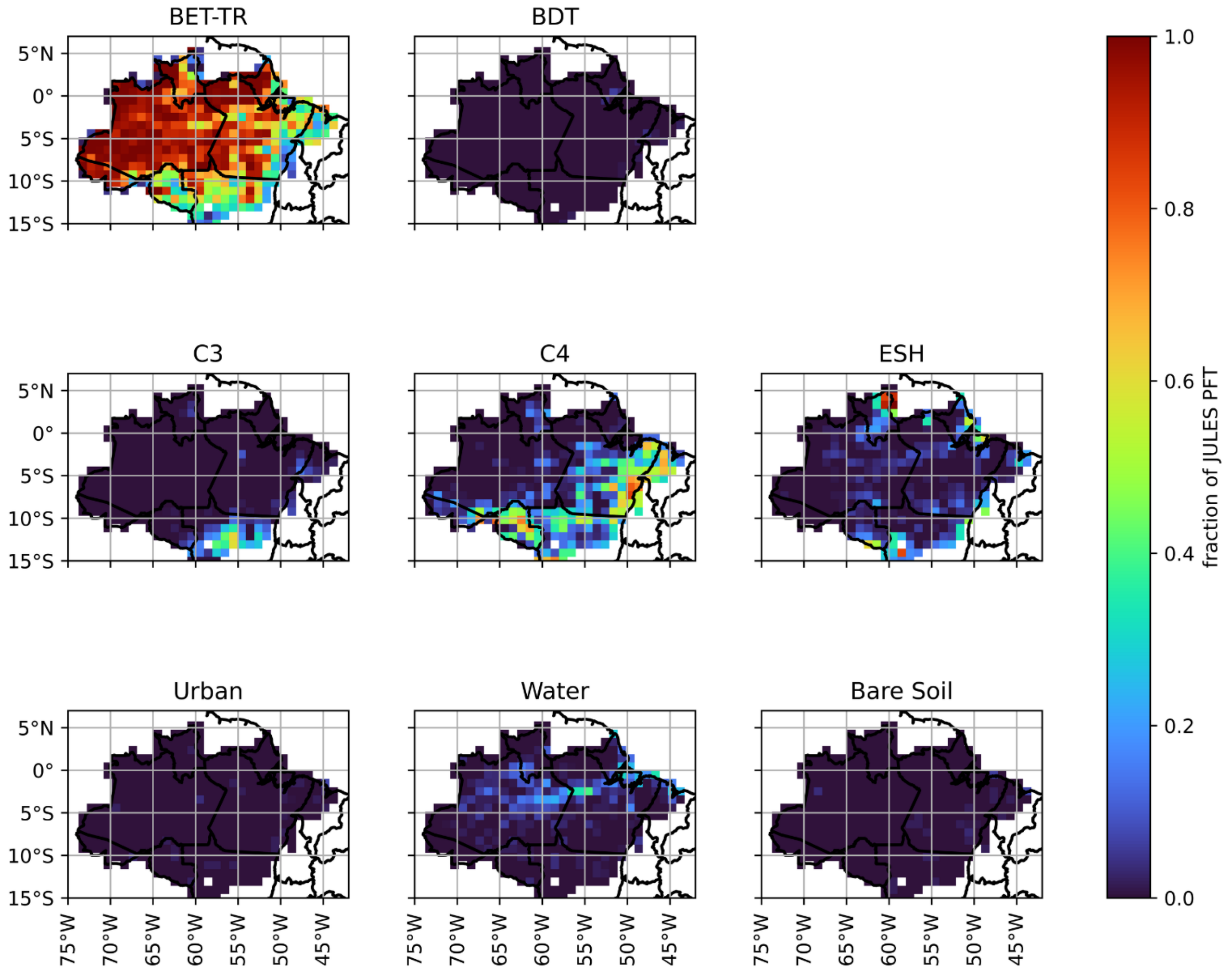

Figure S3.1.1: Distribution of each JULES plant and non-plant functional type in the S3.2.1 utilized for spatializing the carbon flux simulations.

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 S3.2.1). Physically, it makes sense to have an inverse relationship between Tupp and canopy height, since low-canopy plants like 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 values. The 45ºC limit was based in Harper et al., (2016) which defined a Tupp of 45ºC for C4 grasses based on a field experiment in Tapajos. This is higher than the value used by Osborne et al (2015) for soybean (36ºC) and near the Tupp value for Maize (45ºC).. In the forest areas, the parameterization of Tupp using canopy height as predictor result in a range of values from 37ºC , in regions with high canopy height such as in K67 and RJA towers (36 m and 35 m), to 42ºC in 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).

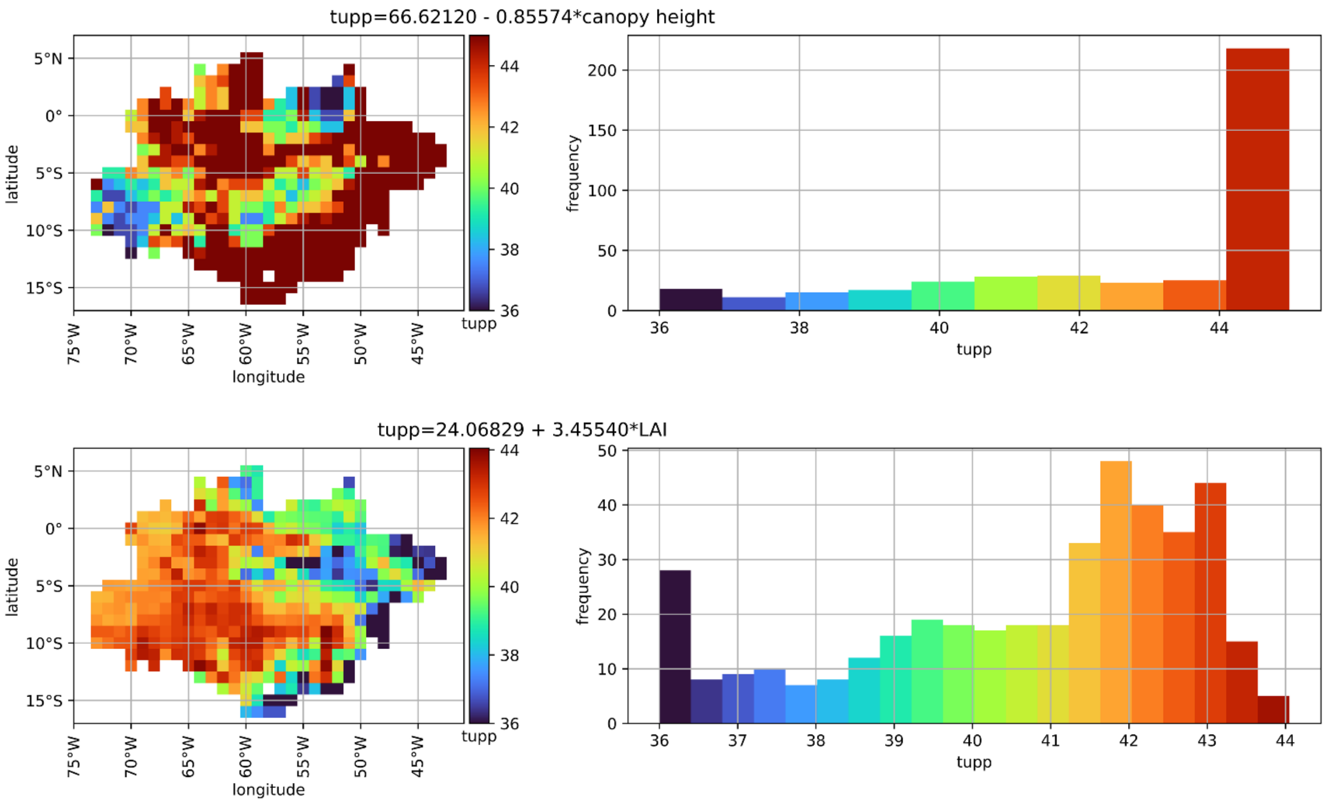

Figure S3.2.1: Tupp spatialized for the Brazilian Amazon biome using two different predictors, canopy height and LAI.

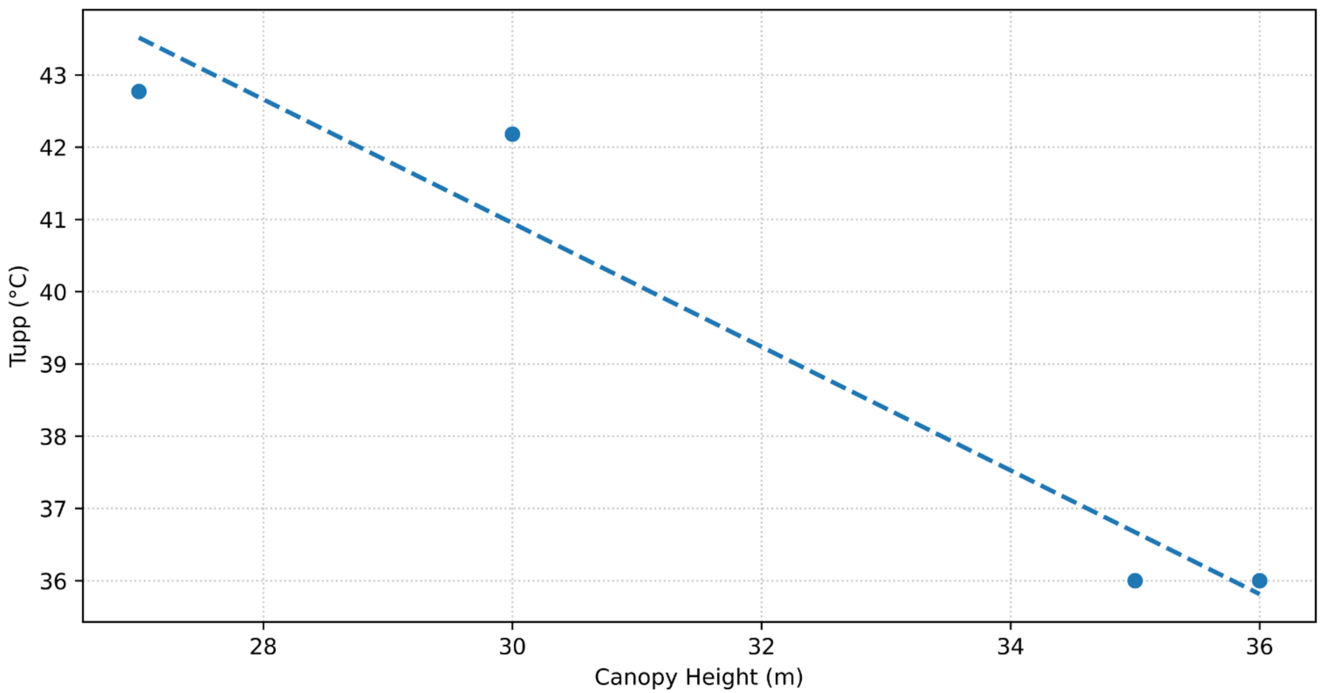

Figure S3.2.2: Relationship between Canopy Height and Tupp (ºC) for different sites of the Brazilian Amazon biome.

S.3.3. alpha, quantum efficiency

Regarding the parameter alpha, the best alternative for spatialization is to use canopy height (Figure S3.3.1), as demonstrated by Harper et al., (2016). Tropical forests are more efficiency in converting PAR into carbon, when compared to C4 plants (Harper et al., 2016). Using the canopy height as predictor, the alpha values for forested regions were in the range 0.05 to 0.06 mol/mol, consistent with Skilmann (2008), who evaluated different species of C3 plants.

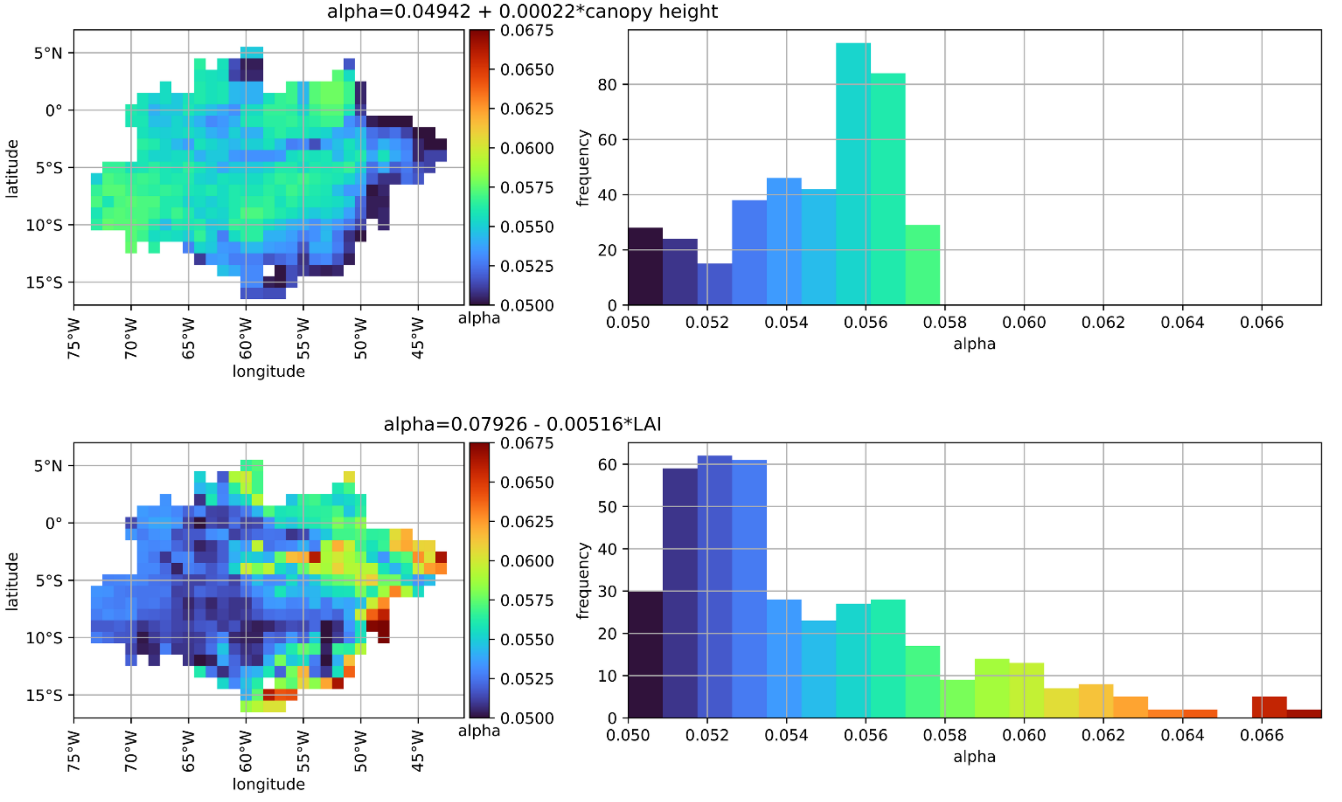

Figure S3.3.1: Alpha spatialized for the Brazilian Amazon biome using two different methods, with canopy height and LAI.

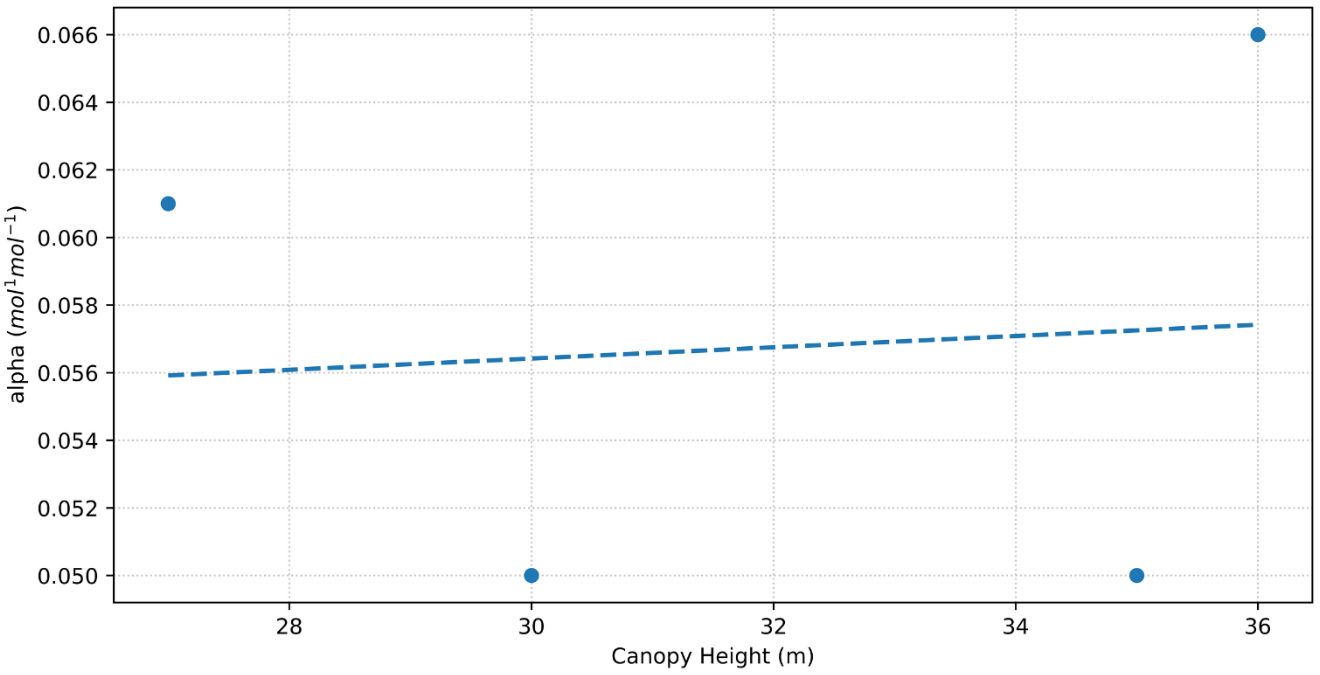

Figure S3.3.2: Relationship between Canopy Height (m) and alpha (mol^1 mol^{-1}) for different sites of the Brazilian Amazon biome.

S.3.4. f0, maximum ratio of internal to external CO2

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 in 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 S3.4.1). This option using LAI is the only one that 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 its 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, in which Santarem and Jaru have species more adaptable to longer dry seasons than in ATTO and Manaus. Accordingly, the parametrization of f0 based on LAI retrieved lower values in Santarem.

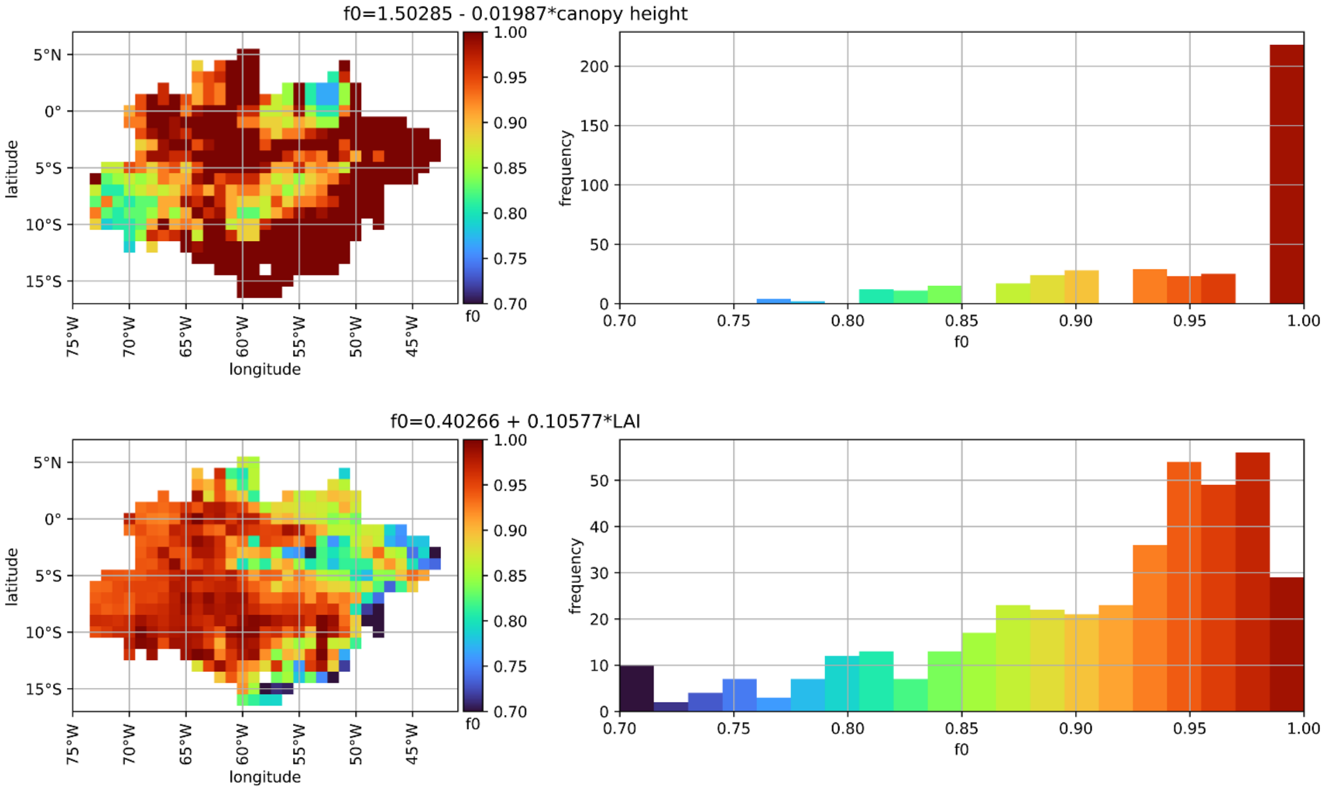

Figure S3.4.1: f0 spatialized for the Brazilian Amazon biome using two different methods, with canopy height and LAI.

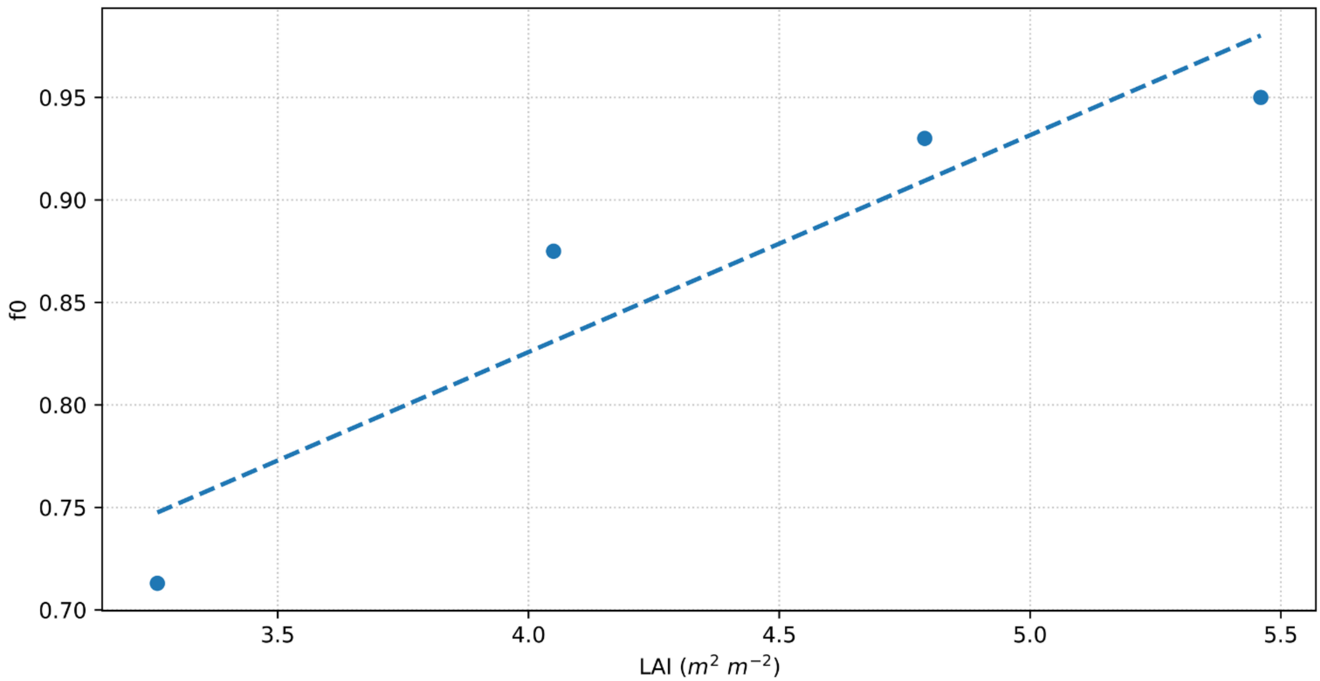

Figure S3.4.2: Relationship between LAI and f0 for different sites of the Brazilian Amazon biome.

S.3.5. fd, scale factor for dark respiration

Like f0, the parameter fd was better represented in the Amazon Basin using LAI (Figure S3.5.1). 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 due to the metabolism that increases carbon concentration in the stomata, reducing the photorespiration. Thus, the parameter fd should be lower for this type of plant than for forest species. Using LAI to extrapolate fd for the Amazon Basin resulted in fd values ranging from 0.005 in the arc of deforestation to 0.015 in forested areas (Figure S6). 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.

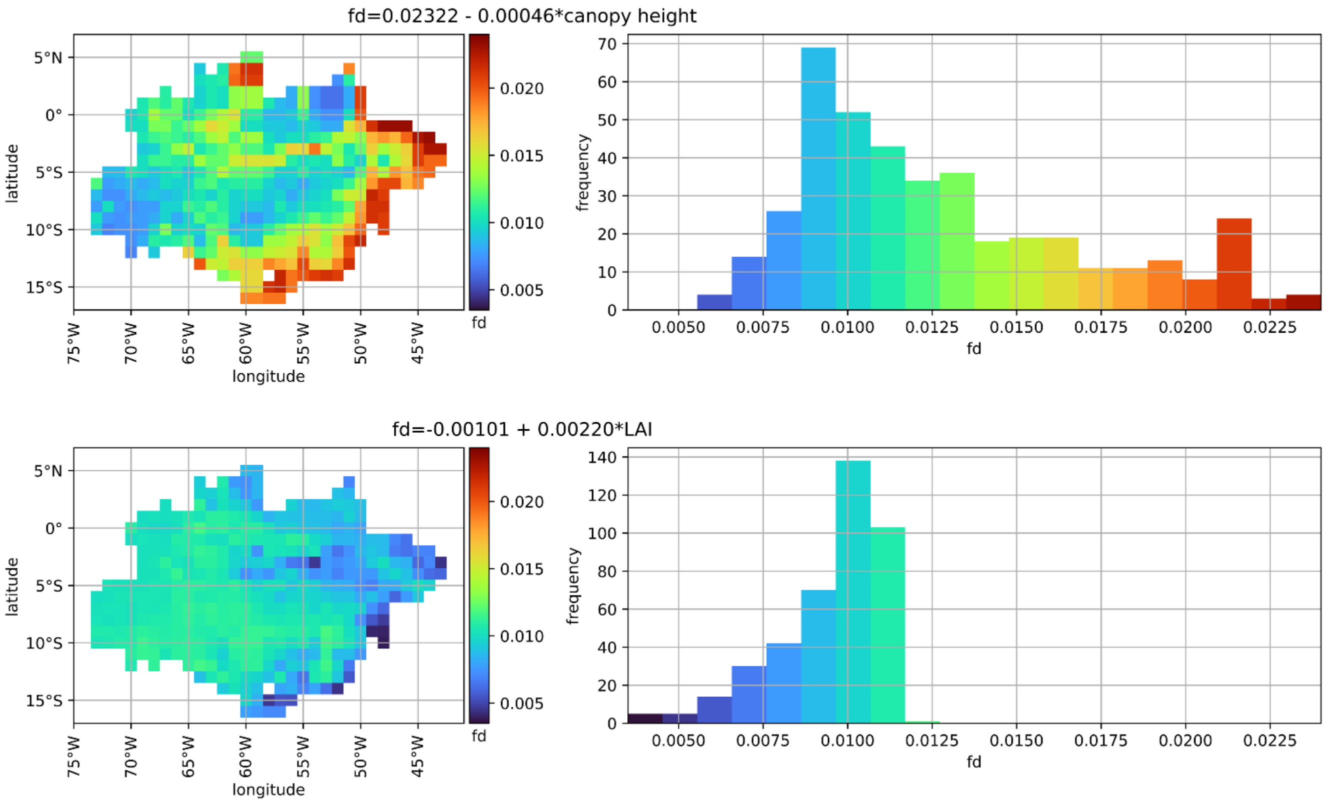

Figure S3.5.1: fd spatialized for the Brazilian Amazon biome using two different methods, with canopy height and LAI.

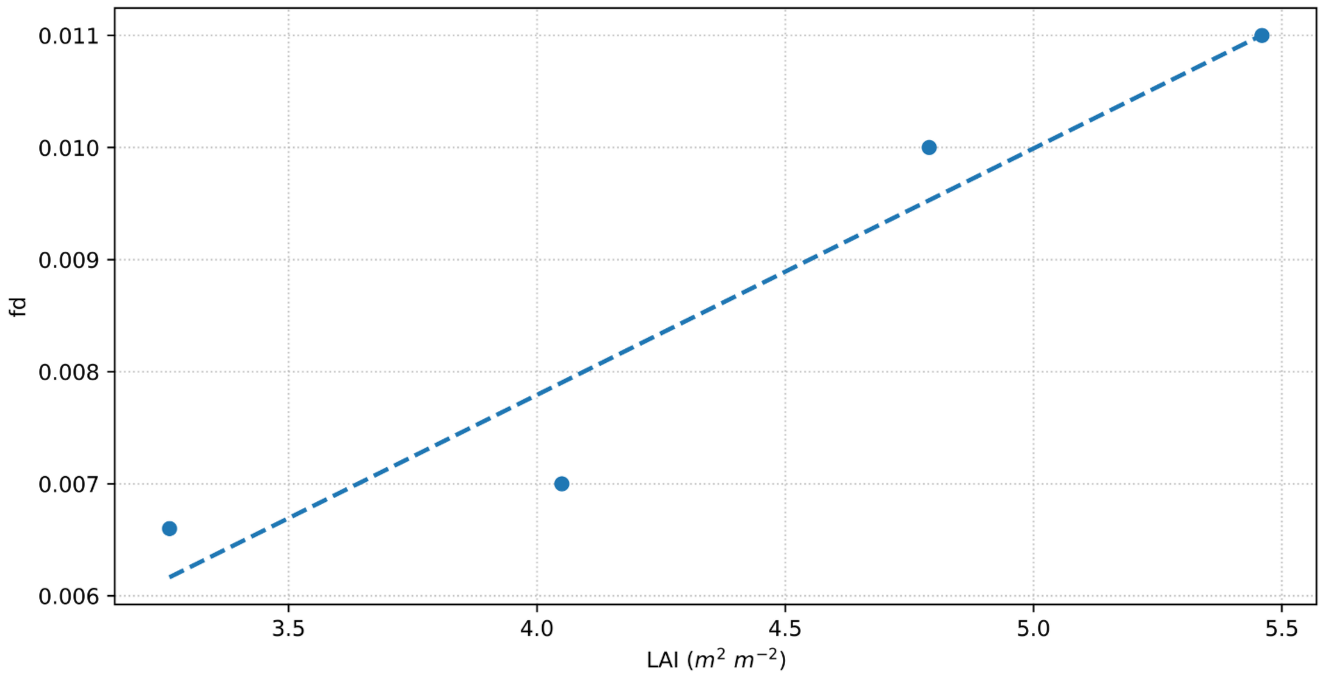

Figure S3.5.2: Relationship between LAI and f0 for different sites of the Brazilian Amazon biome.

S.4. Calibration and evaluation of JULES

Table S4.1: Physiological limits for JULES most sensitivities 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

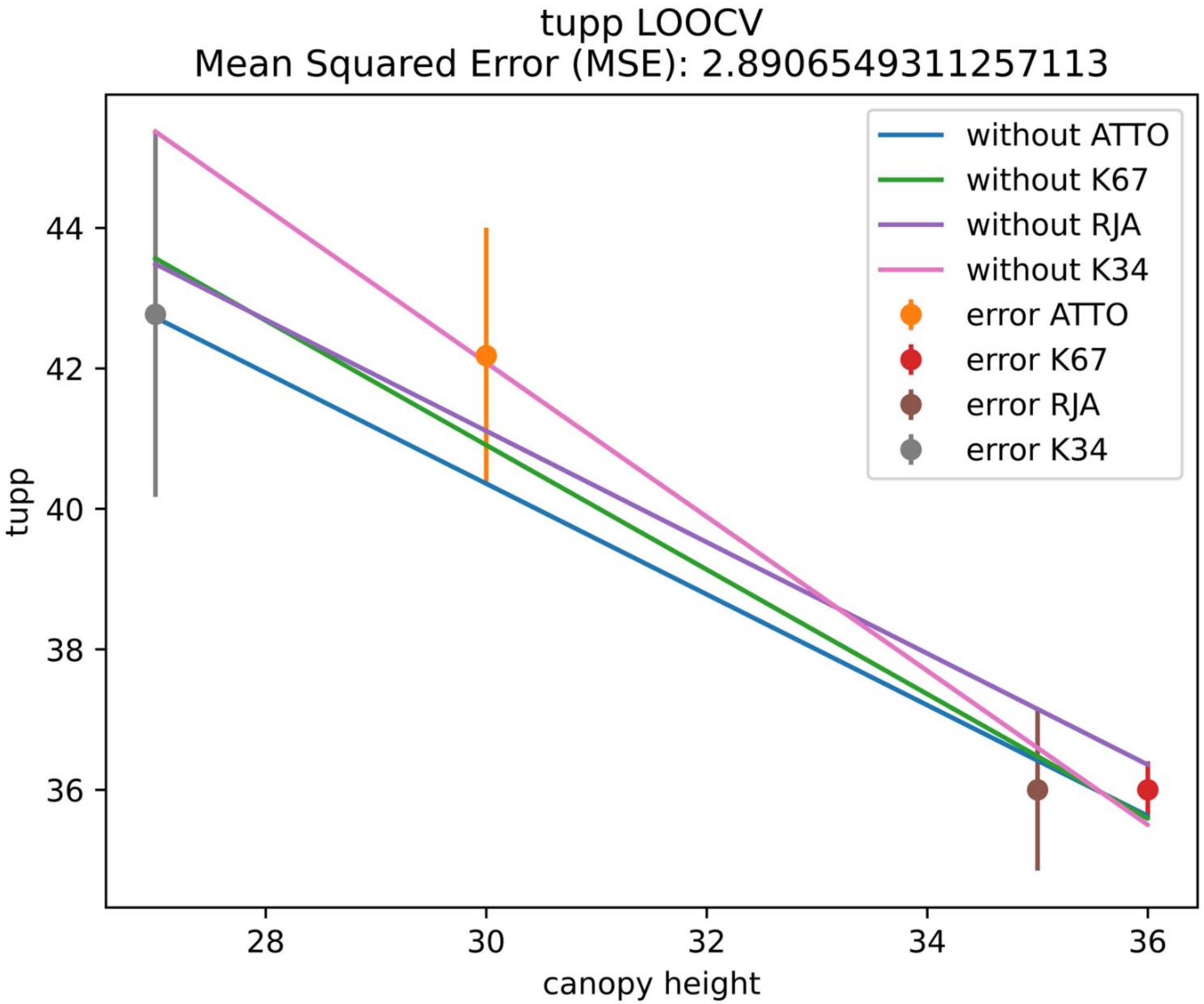

Figure S4.1: Leave-one-out cross-validation (LOOCV) for Tupp in relation to canopy height for four different towers in the Brazilian Amazon biome

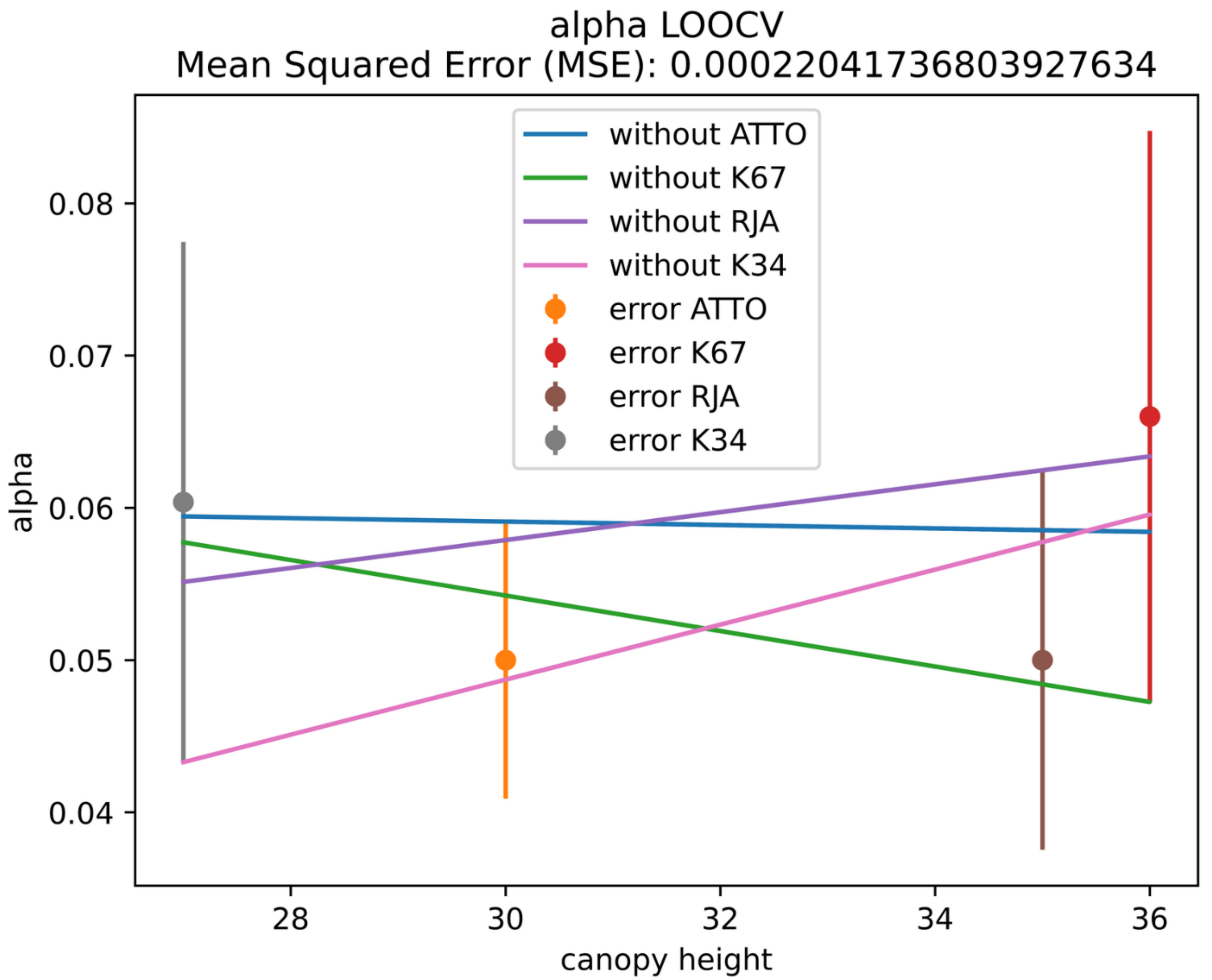

Figure S4.2: Leave-one-out cross-validation (LOOCV) for alpha in relation to canopy height for four different towers in the Brazilian Amazon biome.

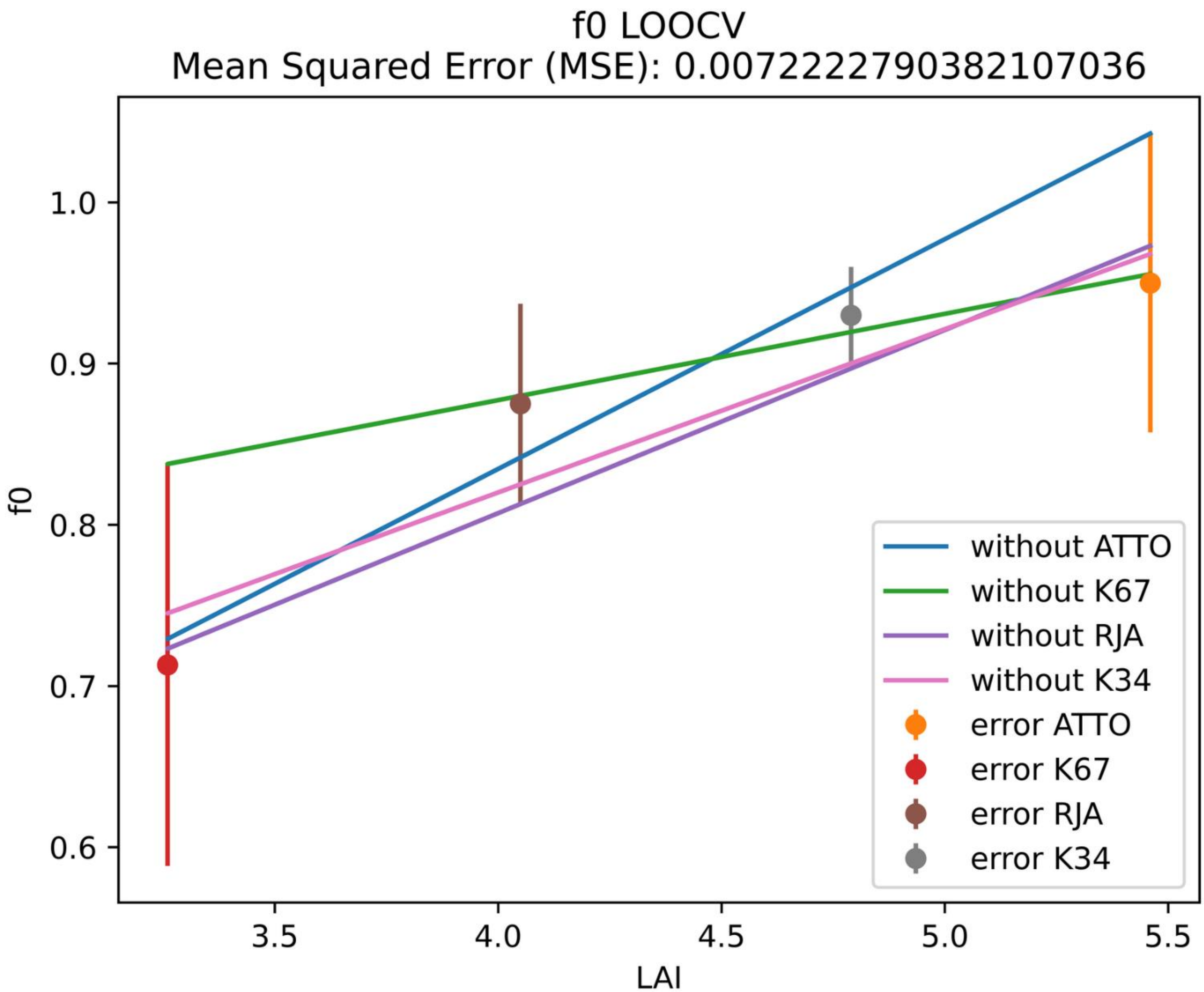

Figure S4.3: Leave-one-out cross-validation for f0 in relation to LAI for four different towers in the Brazilian Amazon biome.

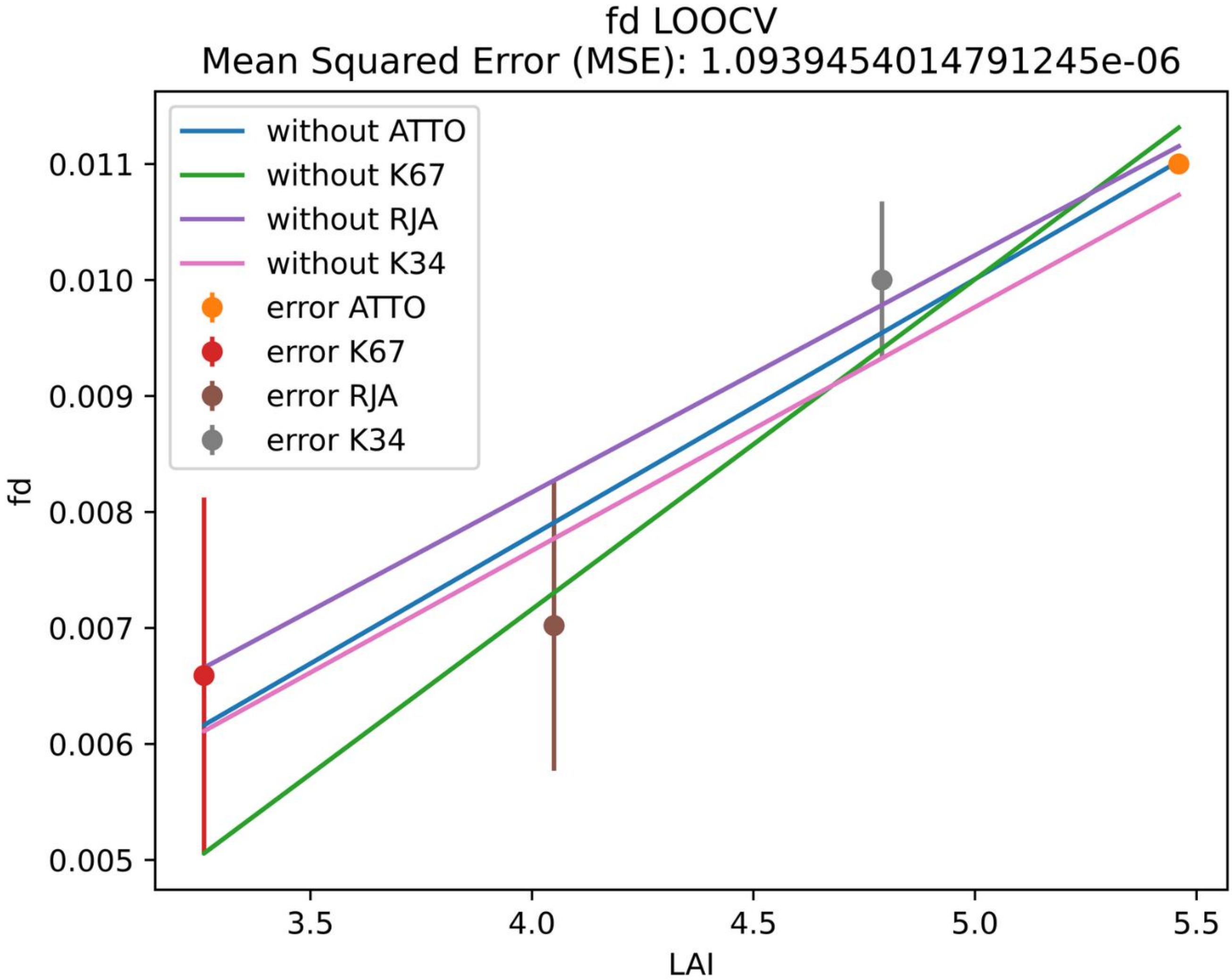

Figure S4.4: Leave-one-out cross-validation for fd in relation to LAI for four different towers in the Brazilian Amazon biome.

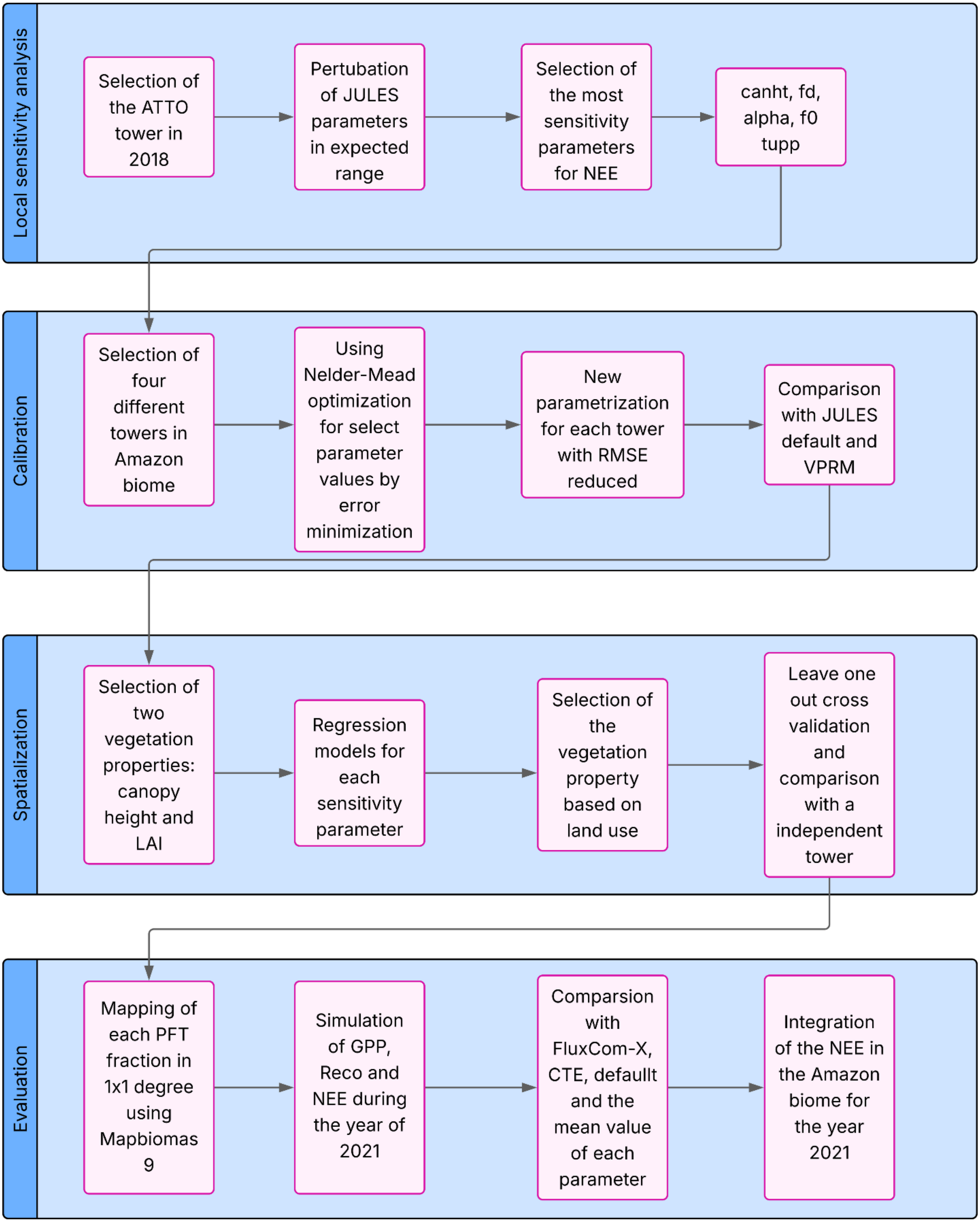
Local sensitivity analysis
Selection of the ATTO tower in 2018
Pertubation of JULES parameters in expected range
Selection of the most sensitivity parameters for NEE
canht, fd, alpha, f0 tupp
Calibration
Selection of four different towers in Amazon biome
Using Nelder-Mead optimization for select parameter values by error minimization
New parametrization for each tower with RMSE reduced
Comparison with JULES default and VPRM
Spatialization
Selection of two vegetation properties: canopy height and LAI
Regression models for each sensitivity parameter
Selection of the vegetation property based on land use
Leave one out cross validation and comparison with a independent tower
Evaluation
Mapping of each PFT fraction in 1x1 degree using Mapbiomas 9
Simulation of GPP, Reco and NEE during the year of 2021
Comparsion with FluxCom-X, CTE, defaullt and the mean value of each parameter
Integration of the NEE in the Amazon biome for the year 2021

Figure S.4.5: Flowchart describing the procedures utilized to spatialize JULES and to obtain the NEE in the Brazilian Amazon biome.

S.5 Comparison with JULES versions

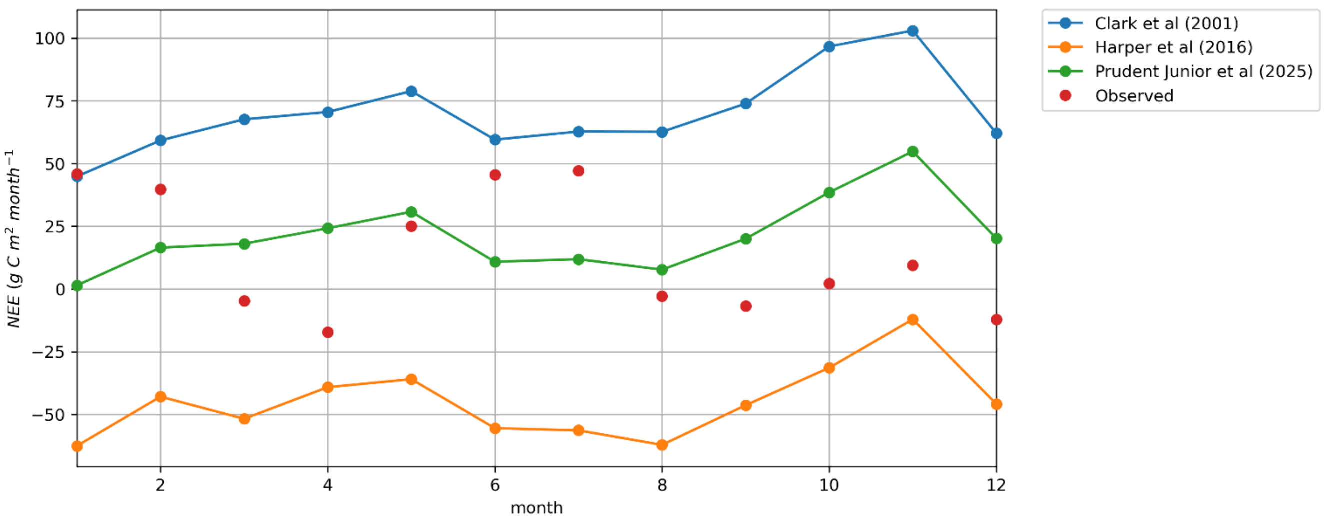

Figure S5. Comparison of NEE simulated in different JULES versions in the ATTO tower during the year of 2018.

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