Supplement S1 - Model optimization

The 6 parameters controlling $Vcmax$, θg and S (Table 1), influencing the GPP values for black spruce, were optimized within a Bayesian framework using observed data at EOBS as reference and Markov Chain Monte Carlo (MCMC) sampling with Metropolis-Hastings steps. The MCMC sampling, through its iterations, only retained the combinations of parameters satisfying the following condition:

$$P_y < e^{(L_y - L_{y-1})}\ ;\ L_y = \prod_{i=1}^{nobs} N(Obs_i;\ \mu = Sim_i, \sigma_y)\, p(\psi_y) \quad \text{(S1)}$$

In Eq. (S1), P_y is a random number between 0 and 1 picked-up at iteration y and L_y is the model posterior probability computed with the product between the model likelihood ($\prod_{i=1}^{nobs} N(Obs_i;\ \mu = Sim_i, \sigma_y)$) and the parameter priors ($p(\psi_y)$). Here we assumed that the model likelihood can be calculated using normal probability densities where Obs_i is an observed GPP daily value, Sim_i is its simulated equivalent and σ_y is the standard deviation of deviations between observation and simulation at iteration y. Moreover, ψ_y is the hyperparameter vector at iteration y composed of the 6 parameters to be optimized plus σ_y. The prior for the 6 parameters was supposed to be uniform over an acceptable range (Table S1), while a Jeffreys prior was used for σ ($\propto 1/\sigma$). In this way, the MCMC sampling maximizes the model posterior probability according to model possibility (i.e. the ability of the model to approximate plausible GPP daily values).

The 12 parameters strongly influencing the MAIDEN Dstem for black spruce (Table 1) were optimized similarly to those 6 influencing GPP. In the computation of the model likelihood (Eq. (S1)), Obs_i was an observed RWhighF value and Sim_i was a simulated detrended yearly Dstem (similarly to RWhighF the detrending was achieved by subtraction by a 10-year cubic smoothing spline). To allow the comparison, both *Obs* and *Sim* were transformed to z-scores. We preferred to optimize MAIDEN on RWhighF values because tree-ring high frequencies are much more robust regionally across sites and trees than low frequencies. Observed and simulated low frequencies were only compared after the optimization of the model parameters.

In the calibration process, to verify the convergence of the sampling, we ran 50 Markov chains starting each time from random initial conditions (i.e. initial values of the parameters in their acceptable ranges). Finally, for each chain, we only selected the iteration with higher model posterior probability. In this way, we got 50 blocks of potential parameters. The convergence of the sampling is shown by the sharp parameters' posterior densities (Figs. S2 and S3) and by the stabilization of the model posterior probability in the 50 chains (Fig. S1). The acceptable ranges (i.e. biologically sound) in which the parameters were sampled are shown in Table S1.

The MAIDENiso GPP is determined by the 6 calibrated parameters (Table 1), but is also influenced by variations in the canopy biomass, which, in part, depend on the values of the parameters controlling the carbon allocation. To avoid that the parameter selection during the MCMC sampling used to calibrate the MAIDENiso GPP was sensitive to the values of the parameters controlling the carbon allocation, we calibrated the 6 GPP parameters fixing the carbon contained in the canopy

reservoir at a constant value. Subsequently, during the calibration of the parameters controlling the carbon allocation, the carbon in the canopy was allowed to vary. In this way, the GPP calibration is independent from the calibration of the carbon allocation, but the parameter selection for the allocation depends on the GPP parameters.

For both the GPP and the carbon allocation, we selected a block of parameters that we called "Plausible Block" ("Plausible Block GPP" and "Plausible Block Stem") and often used to illustrate the results. The selection was based on these criteria:

$$\left(L_y > L_{mode}\right) \,\&\, \left(\sum_{z=1}^{n}\left(ParL_{\psi_{y,z}} \cdot ParRange_z\right) = Maximum\right) \rightarrow \left(\psi_y = Plausible\ Block\right) \quad \text{(S2)}$$

Basically, the model posterior probability with this block of parameters (L_y) must be higher than the mode of the 50 retained iterations (Fig. S1) and the sum of the products between the parameters' posterior probabilities ($ParL$; Figs. S2 and S3) and the spans of their acceptable ranges ($ParRange$) must be maximized. ψ_y is the hyperparameter vector at iteration *y* (here not including σ_y) composed of *n* parameters. The reader should note that the two Plausible Blocks are only a possibility over the retained iterations, which were used to simplify visualizations and interpretations.

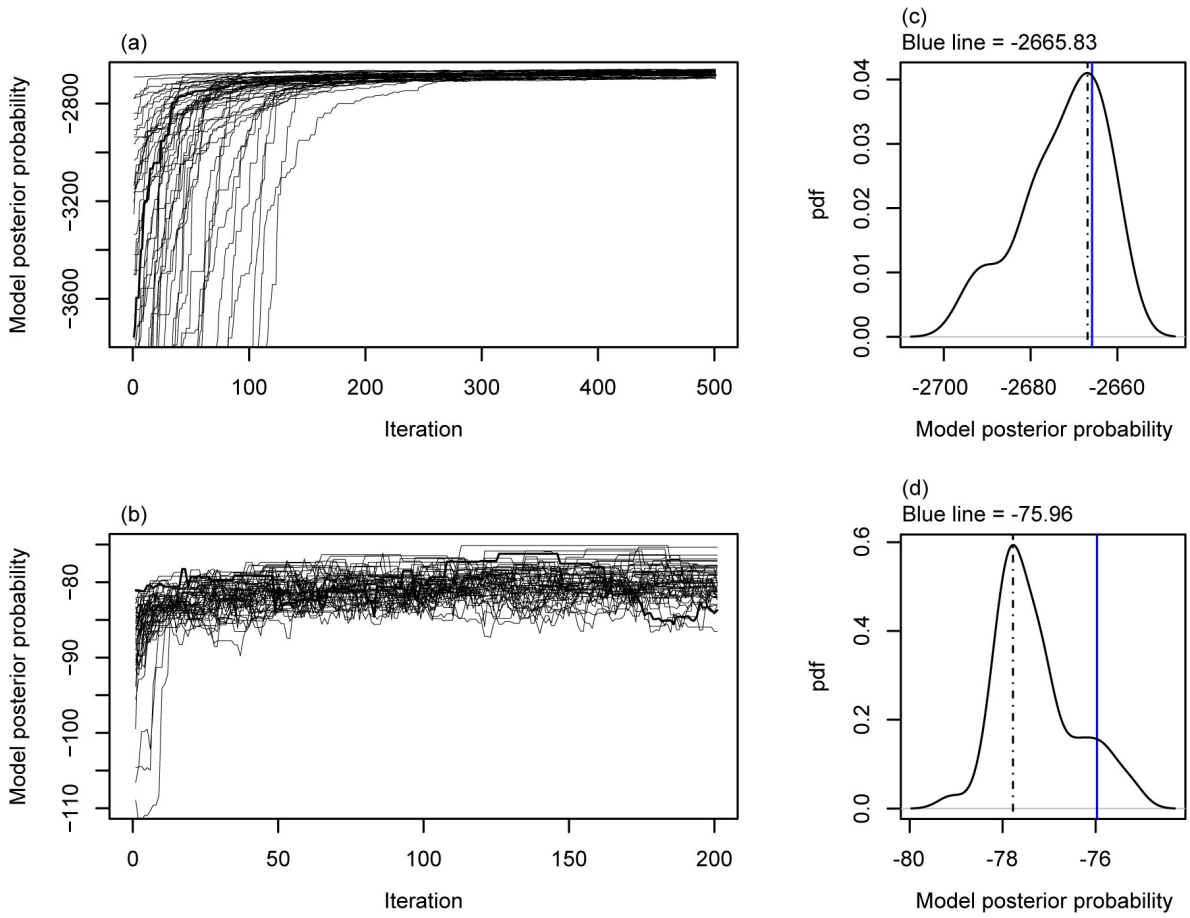

Figure S1: Evolution of the model posterior probability in the 50 Markov chains used in the MAIDENiso calibration. (a) Calibration of GPP (i.e. 6 parameters). (b) Calibration of carbon allocation to the stem (i.e. 12 parameters). Plots (c) and (d) show the model posterior density of the retained 50 blocks of parameters (one block per each chain of (a) and (b)). Vertical dashed line is the mode and blue line is the value with the respective Plausible Block.

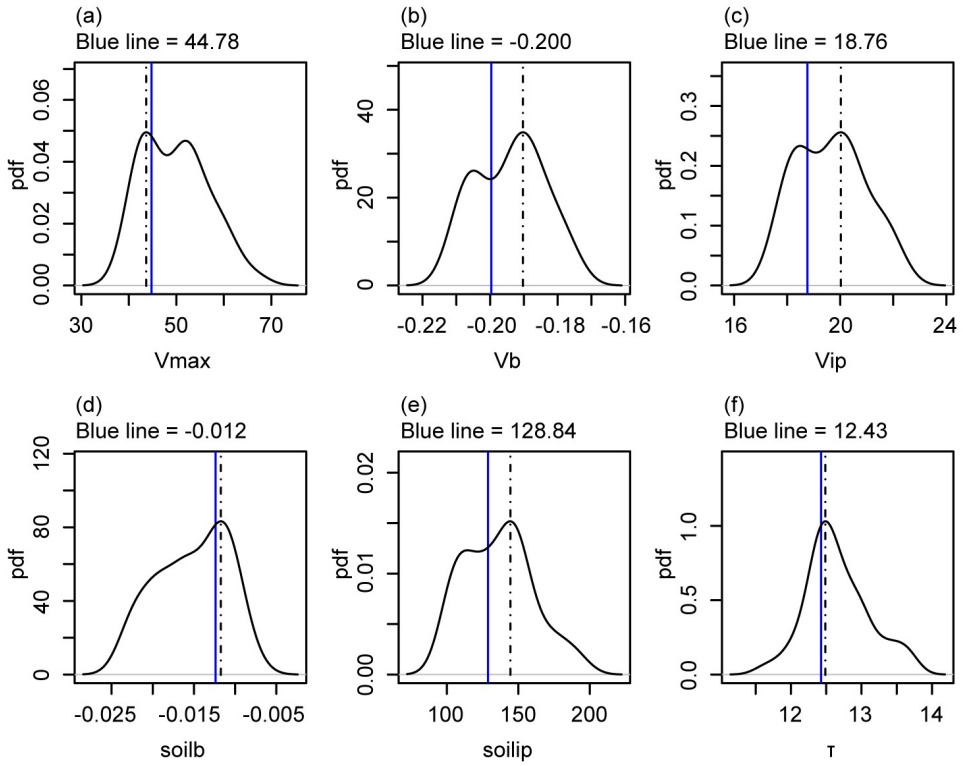

Figure S2: Parameters' posterior densities (pdfs based on 50 values). (a) *Vmax*, (b) *Vb*, (c) *Vip*, (d) *soilb*, (e) *soilip*, and (f) *τ*. Vertical dashed line is the mode and blue line is the value with Plausible Block GPP.

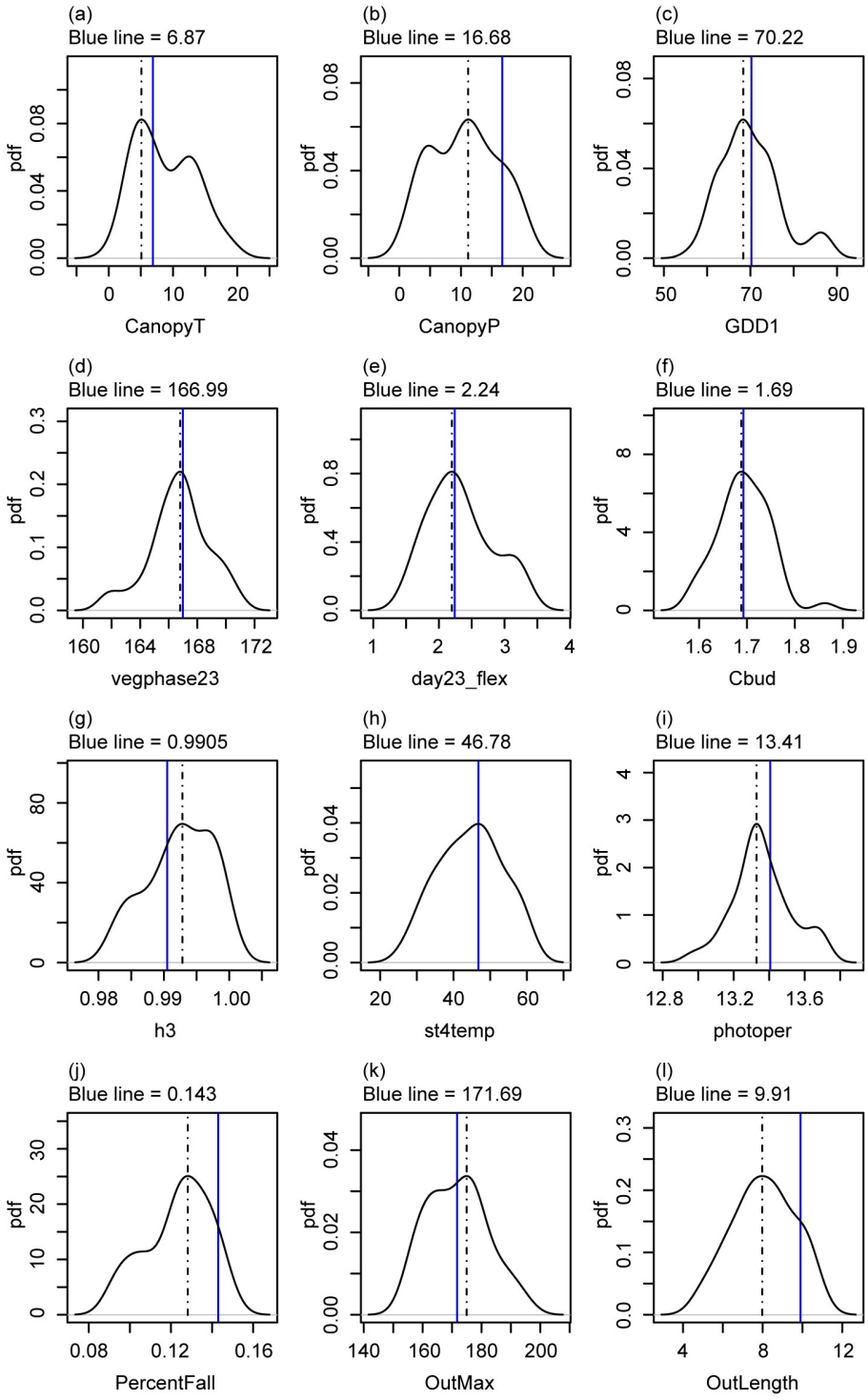

Figure S3: Parameters' posterior densities (pdfs based on 50 values). (a) *CanopyT*, (b) *CanopyP*, (c) *GDD1*, (d) *vegphase23*, *(e) day23_flex*, (f) *Cbud*, (g) *h3*, (h) *st4temp*, (i) *photoper*, (j) *PercentFall*, (k) *OutMax*, (l) *OutLength*. Vertical dashed line is the mode and blue line is the value with Plausible Block Stem.

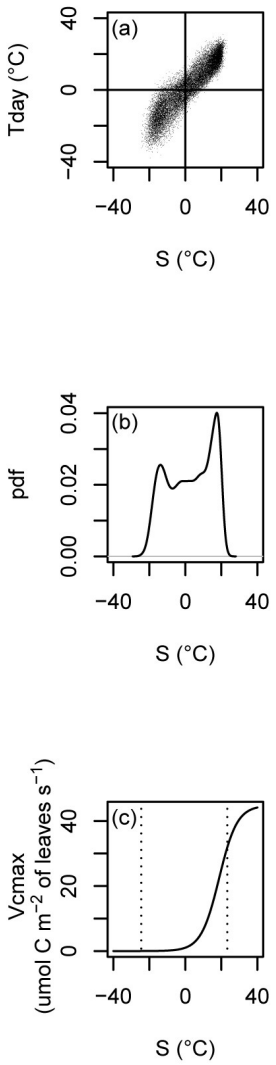

Figure S4: Temperature dependence of maximum carboxylation rate (*Vcmax*) when MAIDENiso is run with the parameters of Plausible Block GPP at the Quebec Eastern Old Black Spruce site (EOBS). (a) Relationship between daytime temperature ($Tday$) and its transformation used in the *Vcmax* equation (*S*). (b) *S* probability density at EOBS. (c) Relationship between *S* and *Vcmax*. The vertical dashed lines show the range of *S* values at EOBS.

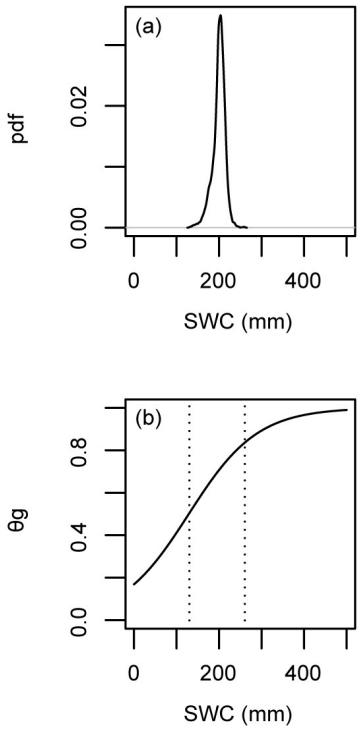

Figure S5: Water stress level (θg) function when MAIDENiso is run with the parameters of Plausible Block GPP at the Quebec Eastern Old Black Spruce site (EOBS). (a) Soil water content (*SWC*) probability density at EOBS. (b) Relationship between *SWC* and θg (higher values correspond to lower stress). The vertical dashed lines show the range of *SWC* values at EOBS.

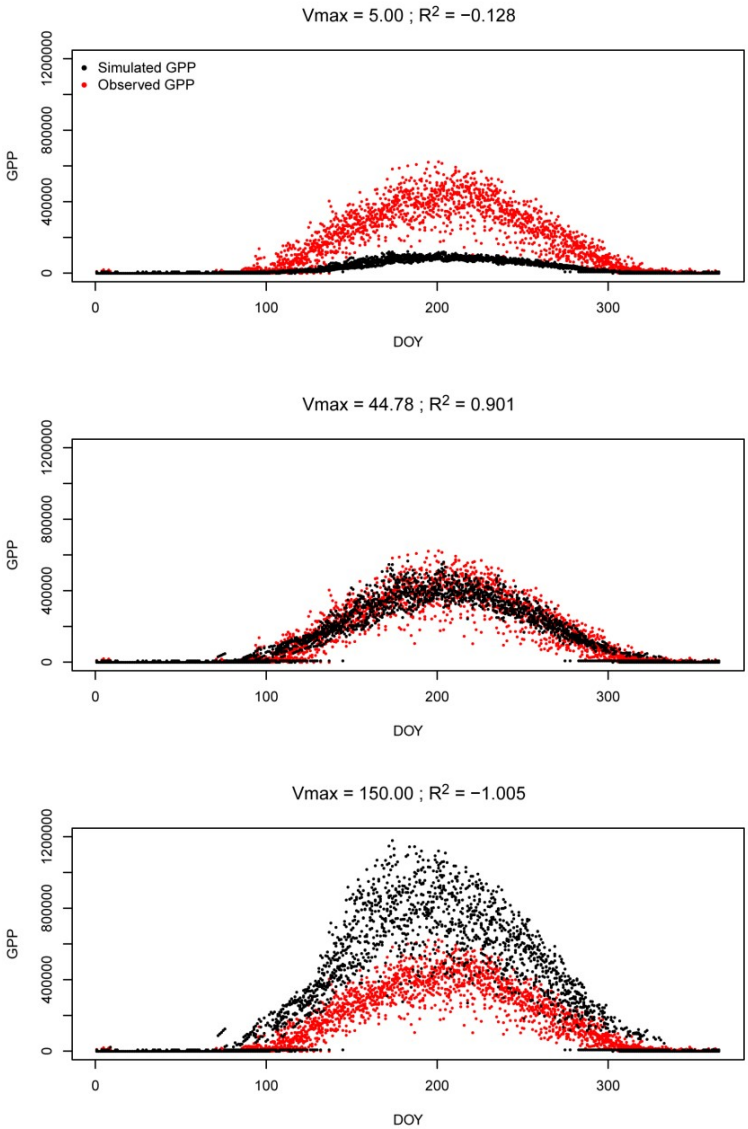

Figure S6: Sensitivity of the daily GPP simulated annual cycle (umol C m^{-2} day^{-1}) to the *Vmax* parameter influencing *Vcmax*. Only *Vmax* varies while the other parameters were fixed to the values of Plausible Block GPP. In the top (bottom) plot, *Vmax* was fixed to the lowest (highest) value of its prior acceptable range. In the middle plot, it was fixed to the selected value for Plausible Block GPP. The R^2 between observations and simulations and the parameter value are reported for each plot.

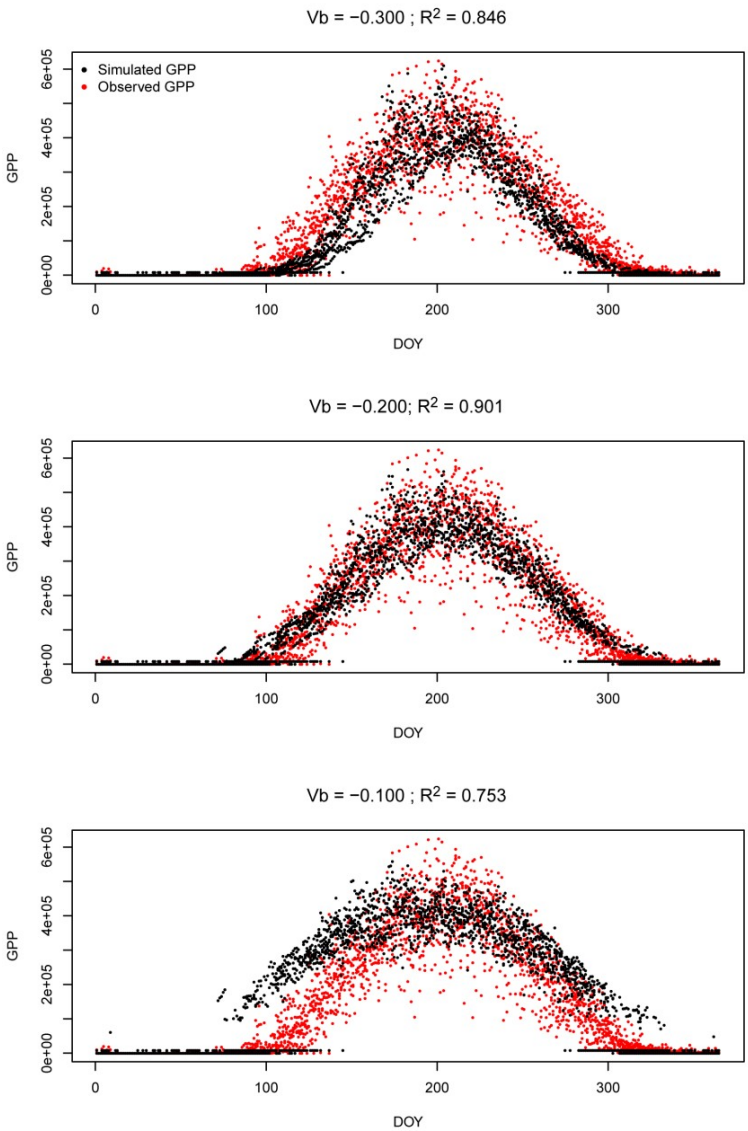

Figure S7: Sensitivity of the daily GPP simulated annual cycle (umol C m^{-2} day^{-1}) to the *Vb* parameter influencing *Vcmax*. Only *Vb* varies while the other parameters were fixed to the values of Plausible Block GPP. In the top (bottom) plot, *Vb* was fixed to the lowest (highest) value of its prior acceptable range. In the middle plot, it was fixed to the selected value for Plausible Block GPP. The R^2 between observations and simulations and the parameter value are reported for each plot.

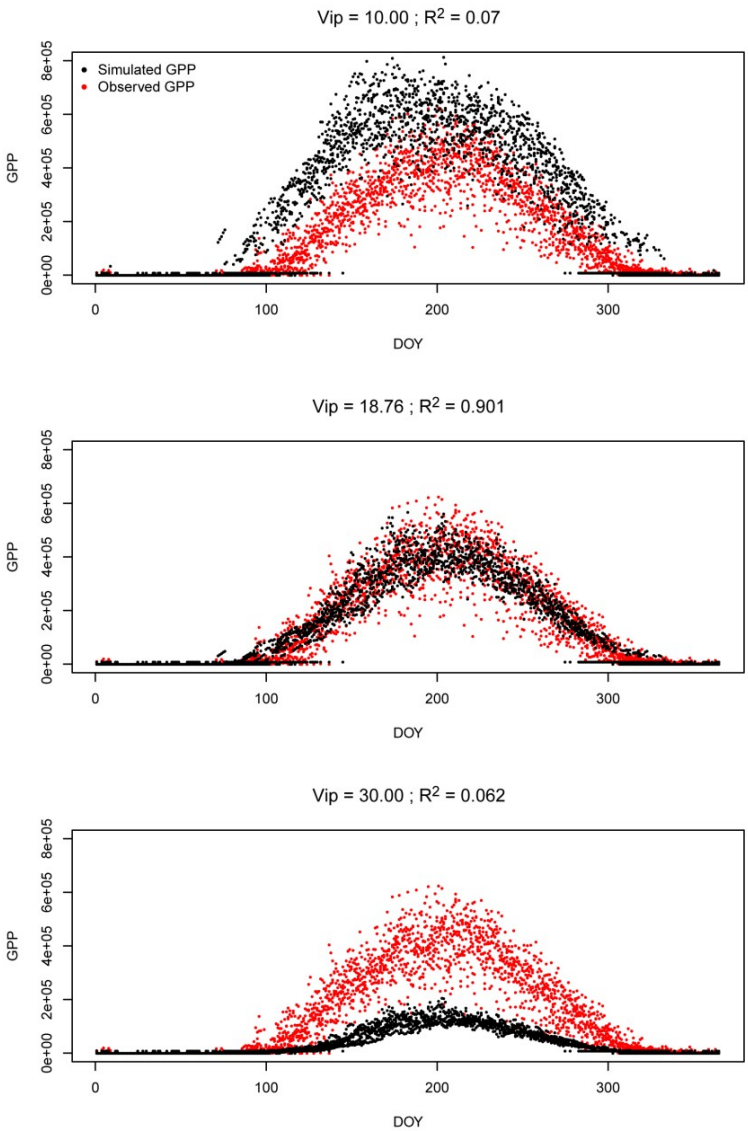

Figure S8: Sensitivity of the daily GPP simulated annual cycle (umol C m^{-2} day^{-1}) to the *Vip* parameter influencing $Vcmax$. Only *Vip* varies while the other parameters were fixed to the values of Plausible Block GPP. In the top (bottom) plot, *Vip* was fixed to the lowest (highest) value of its prior acceptable range. In the middle plot, it was fixed to the selected value for Plausible Block GPP. The R^2 between observations and simulations and the parameter value are reported for each plot.

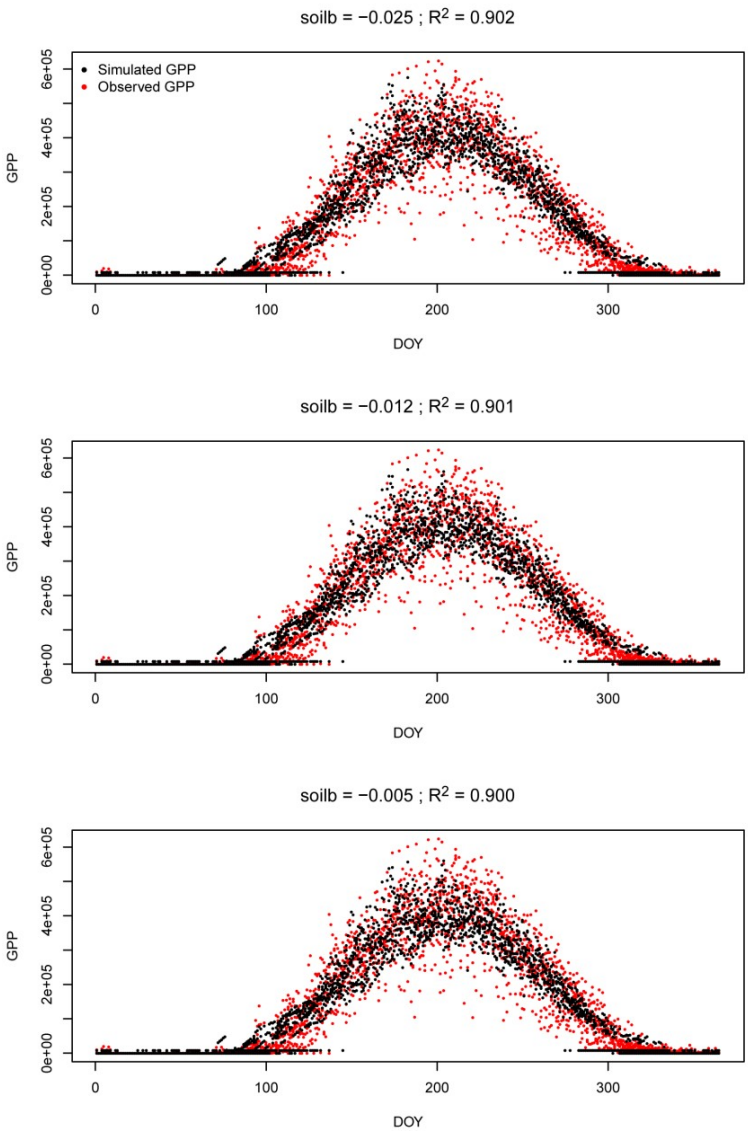

Figure S9: Sensitivity of the daily GPP simulated annual cycle (umol C m^{-2} day^{-1}) to the *soilb* parameter influencing θg.Only *soilb* varies while the other parameters were fixed to the values of Plausible Block GPP. In the top (bottom) plot, *soilb* was fixed to the lowest (highest) value of its prior acceptable range. In the middle plot, it was fixed to the selected value for Plausible Block GPP. The R^2 between observations and simulations and the parameter value are reported for each plot.

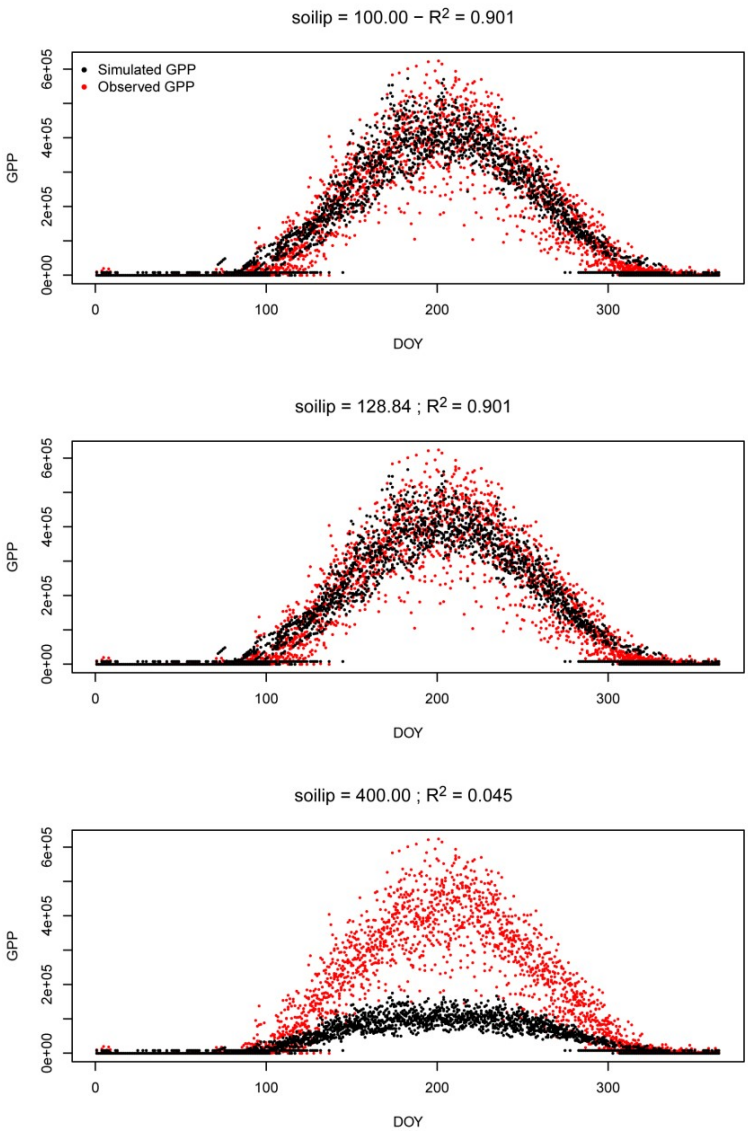

Figure S10: Sensitivity of the daily GPP simulated annual cycle (umol C m^{-2} day^{-1}) to the *soilip* parameter influencing θg. Only *soilip* varies while the other parameters were fixed to the values of Plausible Block GPP. In the top (bottom) plot, *soilip* was fixed to the lowest (highest) value of its prior acceptable range. In the middle plot, it was fixed to the selected value for Plausible Block GPP. The R^2 between observations and simulations and the parameter value are reported for each plot.

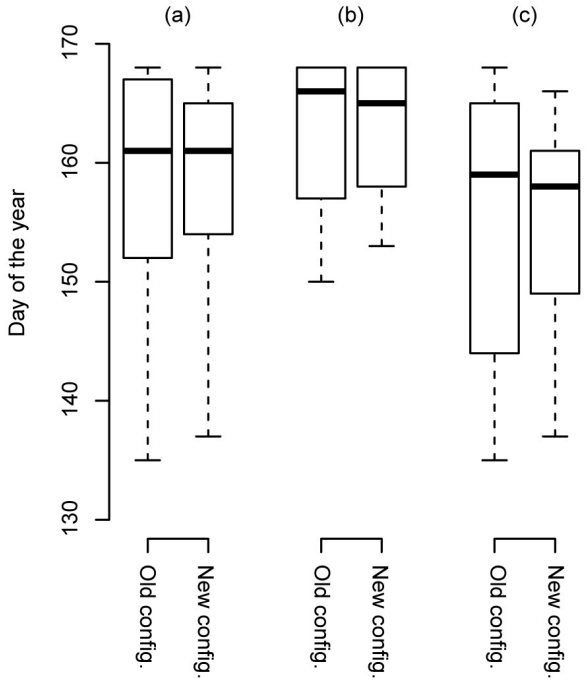

Figure S11: Growing season start (quartiles and extreme values) during the 1950-2010 (a), 1950-1970 (b) and 1990-2010 (c) periods. The parameters of Plausible Block Stem are used with ("New config.") or without ("Old config.") the mechanism to have more smoothed yearly variations.

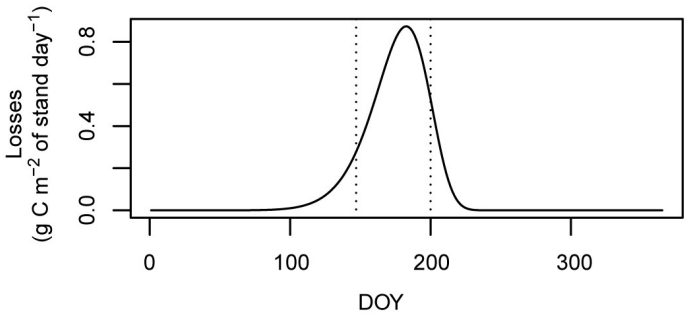

Figure S12: Simulated annual cycle of carbon losses from the canopy (i.e. leaf shedding) when MAIDENiso runs with the parameters of Plausible Block Stem and the potential maximum amount of carbon that the canopy can contain during the year is 307 g C m^{-2} of stand (this value is the average of the simulated *AlloCcanopy*$_j$ values). Vertical dashed lines show the period over which the 80% of the yearly losses are observed.

Table S1: Comparison between prior and posterior ranges of calibrated parameters.

Parameter	Units	Prior Range	Posterior range	Value in Plausible Block
Vmax	umol C m^{-2} of leaves s^{-1}	5 / 150	39 / 67	44.778
Vb	NA	-0.30 / -0.10	-0.21 / -0.17	-0.200
Vip	°C	10 / 30	17.5 / 22.3	18.763
soilb	NA	-0.025 / -0.005	-0.023 / -0.008	-0.012
soilip	mm	100 / 400	102 / 193	128.837
τ	days	1 / 20	11.6 / 13.7	12.428
CanopyT	NA	0 / 20	0.54 / 19.24	6.872
CanopyP	NA	0 / 20	1.70 / 19.85	16.683
GDD1	°C	10 / 120	56.75 / 87.05	70.220
vegphase23	day of the year	152 / 181	161.5 / 171.0	166.988
day23_flex	years	1 / 10	1.53 / 3.29	2.240
Cbud	g C·m^{-2} of stand·day^{-1}	1 / 3	1.59 / 1.86	1.692
h3	fraction (0-1)	0 / 1	0.983 / 1.000	0.991
st4temp	°C	1 / 100	27.53 / 59.11	46.777
photoper	hours	12 / 14	12.96 / 13.72	13.406
PercentFall	fraction (0-1)	0.09 / 0.15	0.093 / 0.149	0.143
OutMax	day of the year	150 / 200	154.2 / 195.0	171.685
OutLength	NA	4 / 12	4.80 / 10.80	9.905