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Bayesian integration of flux tower data into process-based simulator for quantifying uncertainty in simulated output

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Abstract.

Parameters of a process-based forest growth simulator are difficult or impossible to obtain from field observations. Reliable estimates can, however, be obtained using calibration against observations of output and state variables. In this study, we present a Bayesian framework to calibrate the widely used process-based simulator BIOME-BGC against estimates of gross primary production (GPP) data. We used GPP partitioned from flux tower measurements of a net ecosystem exchange over a 55 year old Douglas fir stand as an example. The uncertainties of both the BIOME-BGC parameters and the simulated GPP were estimated. The calibrated parameters leaf and fine root turnover (LFRT), ratio of fine root carbon to leaf carbon (FRC:LC), ratio of carbon to nitrogen in leaf ($C:N_{leaf}$), canopy water interception coefficient (W_{int}), fraction of leaf nitrogen in Rubisco (FLNR), and soil rooting depth (SD) characterize the photosynthesis and carbon and nitrogen allocation in the forest. The calibration improved the root mean square error and enhanced Nash-Sutcliffe efficiency between simulated and flux tower daily GPP compared to the uncalibrated BIOME-BGC. Nevertheless, the seasonal cycle for flux tower GPP was not reproduced exactly, and some overestimate in spring and underestimates in summer remained after calibration. Further analysis showed that, although simulated GPP was time dependent due to carbon allocation, it still followed the variability of the meteorological forcing closely. We hypothesized that the phenology exhibited a seasonal cycle that was not accurately reproduced by the simulator. We investigated this by allowing the parameter values to vary month-by-month. Time varying parameters substantially improved the simulated GPP as compared to GPP obtained with constant parameters. The time varying estimation also revealed a seasonal change in parameter values that determine phenology, and in parameters that determine soil water availability. It was concluded that Bayesian calibration approach can reveal features of the modelled physical processes, and identify aspects of the process simulator that are too rigid.

Keywords: Process-based simulator, BIOME-BGC, gross primary production, Bayesian calibration, uncertainty estimation.

1 Introduction

Forest ecosystems play an important role in the global carbon cycle by controlling atmospheric CO_2 level. Knowledge of gross primary production (GPP) for forest ecosystems is indispensable for the estimation of forest carbon storage. Process-based

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forest simulators (PBS) evaluate forest ecosystem activity by simulating different physiological plant responses to climatic conditions, atmospheric properties and plant structures (Constable and Friend, 2000; Running, 1994).

A PBS requires input parameters that distinguish different vegetation types by their physiological and morphological characteristics. Implementation of a PBS for specific sites is complicated by the large number of parameters for plants, the soil and the atmosphere. Field measurements of PBS parameters are difficult or impossible leading to incomplete knowledge of site specific parameters for the occurring species. In practice practitioners often rely on the literature for values of the PBS parameters (Hartig et al., 2012; Mäkelä et al., 2000).

A systematic adjustment of PBS parameters are required within the margins of the uncertainty so that the simulated outputs (e.g., GPP) satisfy pre-agreed criteria. This adjustment of a simulator parameters is called calibration. Calibration is often performed to obtain single optimized values of the parameters without the quantification of uncertainty in the parameters and the simulated outputs. Quantification of uncertainty is important for both scientific and practical purposes (Bastin et al., 2013; He et al., 2014; Hamm et al., 2015b).

The Bayesian framework provides a coherent method for calibrating a PBS (van Oijen et al., 2011; Reinds et al., 2008; van Oijen et al., 2005) and involves the identification of uncertainty in the parameters from the available information. This uncertainty is expressed as the prior probability distributions of the parameters. Independent observations of the variables corresponding to the PBS outputs (e.g., GPP) are used to update the prior probability distributions by means of Bayes rule. This updating generates the posterior probability distributions of the parameters, which can be summarized as medians and 95% credible intervals as the quantification of uncertainty. Hence the Bayesian framework combines prior probability distributions of the parameters and the observations to quantify uncertainty in the parameters and the PBS outputs.

In this study, a widely used simulator BIOME-BGC (Thornton, 1998) was calibrated in a Bayesian framework for the single output variable, GPP. A systematic search of the literature was used to construct the prior probability distributions on the BIOME-BGC parameters (Raj et al., 2014). A time series of daily flux tower GPP, which had been partitioned from the flux tower measurements of net ecosystem exchange, provided independent observations of GPP (Raj et al., 2016). We used flux tower GPP to update the priors of BIOME-BGC parameters. BIOME-BGC simulates GPP at daily time-step and it updates its memory between days (Thornton, 2010; White et al., 2000). This memory corresponds to the mass (amount of carbon) stored in different components of the vegetation, litter, and soil. This study further investigated the effect of BIOME-BGC memory to reproduce the seasonal cycle of GPP by means of Bayesian calibration.

The objective of this study was to quantify the uncertainty in BIOME-BGC input parameters and simulated GPP by integrating flux tower GPP into BIOME-BGC in a Bayesian framework. We obtained the posterior BIOME-BGC parameters: a) that do not vary over the entire study period; and b) that vary at the monthly time-steps. The monthly variation in posterior parameters allowed us to 'overrule' the simulated mass storage by those of a simulation with different parameter values. This enabled us to evaluate which part of the memory of the BIOME-BGC needs improvement.

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2 Site description

Calibration of BIOME-BGC was performed at the Speulderbos forest site, which is located at $52^o15'08''$ N, $05^o41'25''$ E within a large forested area in the Netherlands. There is a flux tower within a dense 2.5 ha Douglas fir stand, which is a type of evergreen needleleaf species. The stand was planted in 1962. The vegetation, soil, and climate of this site have been thoroughly described elsewhere (Su et al., 2009; van Wijk et al., 2001; Steingrover and Jans, 1994; Raj et al., 2014).

3 Methods

3.1 Data and simulators

3.1.1 The BIOME-BGC simulator

BIOME-BGC simulates biogeochemical processes including carbon, water and nitrogen fluxes within the vegetation, litter and soil compartment of terrestrial ecosystem at a daily time steps (Running and Hunt, 1993; Thornton et al., 2002). Evapotranspiration (ET), photosynthesis and respiration (autotrophic and heterotrophic) are the main processes simulated by BIOME-BGC. Simulation of daily ET is based on the Penman-Monteith equation (Monteith and Unsworth, 2008; McNaughton and Jarvis, 1983), which simulates ET as a function of incoming radiation, vapour pressure deficit (VPD) and the conductance associated with the evaporative surface. The photosynthetic routine uses Farquhar's biochemical model to estimate GPP (Farquhar et al., 1980; Thornton et al., 2002), which is the overall fixation of carbon. GPP is estimated independently for the sunlit and shaded canopy fractions. Final GPP is the sum of the contributions of the sunlit and shaded canopy fractions. GPP is a function of temperature, vapour pressure deficit, soil water content, solar radiation, atmospheric CO_2 concentration, leaf area index and leaf nitrogen concentration (Churkina and Running, 1998). The photosynthesis routine adds carbon to the system, which is removed from the system through respiration. Respiration routine computes autotrophic respiration as the sum of maintenance and growth respiration. Maintenance respiration is calculated as a function of leaf and root nitrogen concentration and tissue temperature. Growth respiration is the proportion of total new carbon allocated to growth. Heterotrophic respiration is the release of carbon through the process of decomposition of both litter and soil.

BIOME-BGC requires site characteristics, daily meteorological data, and ecophysiological parameters as inputs. The site characteristics include soil texture (percentage of sand, silt, and clay), elevation, latitude, shortwave albedo, wet and dry atmospheric deposition of nitrogen, symbiotic and asymbiotic fixation of nitrogen, and the effective soil rooting depth. We took the site characteristics data at Speulderbos from Raj et al. (2014). The meteorological data include daily minimum temperature (Tmin), daily maximum temperature (Tmax), the average daytime temperature (Tday), daily total precipitation, the daylight average shortwave radiant flux density (srad), the daylight average vapour pressure deficit (VPD) and the daylength from sunrise to sunset. We collected half-hourly temperature, prcp, srad, and relative humidity (RH) for each day in 2009 from the Speulderbos flux tower and daily values were obtained by the half hourly measurements. We derived VPD from relative humidity (RH) using the procedure described in Monteith and Unsworth (1990). BIOME-BGC requires 35 ecophysiological

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parameters for evergreen needleleaf forest/species (Table 1) and we obtained the prior uncertainty (expressed as a probability distribution) in each parameter for Speulderbos from Raj et al. (2014).

3.1.2 Flux tower GPP data

We used daily observed data of net ecosystem exchange NEE to predict GPP at Speulderbos for the growing season (April to October) of 2009. To predict GPP, half-hourly GPP were separated from flux tower measurements of half-hourly net ecosystem exchange at Speulderbos site using non-rectangular hyperbola (NRH) model (Gilmanov et al., 2003). The estimation of the NRH model parameters was performed in a Bayesian framework that yielded posterior distributions of the NRH parameters and posterior predictions of GPP and its associated uncertainty (see Raj et al., 2016, for details). NEE was measured every half hour, leading to half-hourly predictions of GPP. These half-hourly values were summed to yield daily values of GPP and its associated uncertainty.

3.2 Bayesian modelling

3.2.1 Bayes rule

Bayesian calibration begins with Bayes rule (Gelman et al., 2013):

$$p(\boldsymbol{\theta}|\mathbf{z}) = \frac{p(\mathbf{z}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{z})} \propto \text{likelihood} \times \text{prior}. \quad (1)$$

The terms in Equation 1 are:

- $p(\boldsymbol{\theta})$ is the prior probability density function (pdf) of the PBS parameters (e.g., FLNR, soil depth), contained in the vector $\boldsymbol{\theta}$;
- $p(\mathbf{z}|\boldsymbol{\theta})$ is the conditional probability of observing the data $\mathbf{z}$ given $\boldsymbol{\theta}$ and is called the likelihood function. The vector $\mathbf{z}$ contains the independent observations of GPP, separated from NEE (see Section 3.1.2);
- $p(\mathbf{z})$ is the normalization constant, which is independent of $\boldsymbol{\theta}$;
- $p(\boldsymbol{\theta}|\mathbf{z})$ is the posterior pdf of $\boldsymbol{\theta}$ given the observed data.

The likelihood function is determined by the probability distribution of the residuals $\mathbf{e} = (e_1, e_2, ..., e_n)$, which are the difference between $\mathbf{y} = (y_1, y_2, .., y_n)$ and $p(\mathbf{z})$:

$$e_t = z_t - y_t, \quad t = 1, 2, ..., n \quad (2)$$

where $\mathbf{y}$ denotes the simulated GPP (i.e., the output from the PBS). The residuals include the observation error and the simulator inadequacy, which arises due to the fact that the simulated output does not represent the true value of the process even if $\boldsymbol{\theta}$ are known with no uncertainty (Kennedy and O'Hagan, 2001).

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The posterior pdf in Eq. (1) cannot be obtained analytically for most practical problems. Inference is performed using the unnormalized density (Gelman et al., 2013) using Markov chain Monte Carlo (MCMC) simulation (Vrugt, 2016; Gelman et al., 2013; Vrugt et al., 2009; Gelfand and Smith, 1990; Hastings, 1970; Metropolis et al., 1953), as described in Section 3.2.2.

3.2.2 DiffeRential Evolution Adaptive Metropolis (DREAM)

We adopted the DREAM algorithm proposed by Vrugt et al. (2009, 2008) to implement MCMC. DREAM stands for DiffeRential Evolution Adaptive Metropolis. DREAM runs N different Markov chains in parallel for each θ_j. Let the vector of simulator parameters $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3, ..., \theta_d)$. The current state of the i^{th} chain is given by single d-dimensional parameter vector $\boldsymbol{\theta}^{(i)}$. The N Markov chains make N such vectors $\boldsymbol{\theta}^{(1)}$, $\boldsymbol{\theta}^{(2)}$,....., $\boldsymbol{\theta}^{(N)}$. The following steps explain briefly the DREAM algorithms.

1. For each chain i ($i = 1, 2, ..., N$), an arbitrary starting point $\boldsymbol{\theta}^{(i)}$ from the prior pdf of the parameters are sampled.

2. A simulator is run at the starting points and and the likelihood $p(\mathbf{z}|\boldsymbol{\theta}^{(i)})$ ($i = 1, 2, ..., N$) is obtained. The density $p(\boldsymbol{\theta}^{(i)}|\mathbf{z})$ is then obtained for each chain:

$$\begin{aligned} p(\boldsymbol{\theta}^{(i)}|\mathbf{z}) &= p(\boldsymbol{\theta}^{(i)}) \times p(\mathbf{z}|\boldsymbol{\theta}^{(i)}) \\ &= \left\{ p(\theta_1^{(i)}) \cdot p(\theta_2^{(i)}) \cdot .... \cdot p(\theta_d^{(i)}) \right\} \times p(\mathbf{z}|\boldsymbol{\theta}^{(i)}) \end{aligned} \tag{3}$$

   The choice of likelihood and prior pdf of $\boldsymbol{\theta}$ for BIOME-BGC are explained in Sections 3.3.2 and 3.3.1.

3. For i = 1,2,3,.....,N:

   (a) A candidate point $\boldsymbol{\theta}^{(i)*}$ in chain i is generated from the randomly chosen pairs of chains:

$$\boldsymbol{\theta}^{(i)*} = \boldsymbol{\theta}^{(i)} + (\mathbf{1}_d + \boldsymbol{\lambda}_d)\gamma(\delta, d) \left(\sum_{k=1}^{\delta} \boldsymbol{\theta}^{(k)} - \sum_{l=1}^{\delta} \boldsymbol{\theta}^{(l)} \right) + \boldsymbol{\zeta}_d \tag{4}$$

   and

$$\gamma = 2.38/\sqrt{2\delta d}$$

   where δ is the number of chain pairs used to generate the candidate point, $\boldsymbol{\theta}^{(k)}$ and $\boldsymbol{\theta}^{(l)}$ are randomly selected from the state of other chains; $k, l \in (1, 2, .., N)$ and $k \neq l \neq i$. The values of $\boldsymbol{\lambda}_d$ and $\boldsymbol{\zeta}_d$ are sampled from the uniform distribution $U(-b, b)$ and the normal distribution $\mathcal{N}(0, c)$ respectively. The typical default values of $\delta = 3$, $b = 1$, and $c = 10^{-6}$. γ is the jump-size, whose value depends on δ and d. DREAM implements a randomized subspace sampling, i.e., all dimensions of $\boldsymbol{\theta}^{(i)}$ are not updated jointly and some dimensions of $\boldsymbol{\theta}^{(i)*}$ are reset to those of $\boldsymbol{\theta}^{(i)}$. The value of γ is, therefore, obtained with d', the number of dimensions updated jointly.

   (b) The simulator is run at the candidate point $\boldsymbol{\theta}^{(i)*}$ and the density $p(\boldsymbol{\theta}^{(i)*}|\mathbf{z}) = p(\boldsymbol{\theta}^{(i)*}) \times p(\mathbf{z}|\boldsymbol{\theta}^{(i)*})$.

   (c) The Metropolis ratio is given as $p(\mathbf{z}|\boldsymbol{\theta}^{(i)*})/p(\mathbf{z}|\boldsymbol{\theta}^{(i)})$

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(d) The candidate point $\boldsymbol{\theta}^{(i)*}$ is accepted if the Metropolis ratio is larger than an acceptance criterion, which is a random number generated from the uniform distribution between 0 and 1. This may allow acceptance of $\boldsymbol{\theta}^{(i)*}$ with a lower likelihood than the current candidate point.

(e) If the candidate point is accepted: $\boldsymbol{\theta}^{(i)} = \boldsymbol{\theta}^{(i)*}$, otherwise it remains at $\boldsymbol{\theta}^{(i)}$.

4. All N Markov chains evolve in parallel for T times by repeating Step 3. In order to perform inference using the Markov chains it is important that the chains have converged to a stationary distribution that is independent of their initial values. This is evaluated using diagnostic statistics and diagnostic plots, as described in Section 3.3.3. Unconverged chains chains are discarded as "burn-in" and the post burn-in samples are then used to conduct inference on each θ_j. The post burn-in samples are then used to conduct inference on each θ_j. For example median and 95 % credible interval can be obtained over these samples. A simulator is run on the posterior distributions of $\boldsymbol{\theta}$ to get the uncertainty in the simulated output (e.g., GPP for BIOME-BGC).

   The choice of N, T, and burn-in period are discussed in Section 3.3.3. The convergence diagnostic of Markov chains are also explained further in Section 3.3.3.

3.3 Implementation of DREAM for BIOME-BGC

3.3.1 Prior distributions of the BIOME-BGC parameters

The computational load of Bayesian calibration of a simulator can be reduced by excluding those input parameters that have negligible influence on the simulated output (Minunno et al., 2013; van Oijen et al., 2013; Xenakis et al., 2008). BIOME-BGC requires 35 ecophysiological parameters for evergreen needleleaf species (Table 1), each having a varying degree of influence on the simulated GPP. Raj et al. (2014) conducted variance-based sensitivity analysis (VBSA) of BIOME-BGC at Speulderbos to investigate the sensitivity of simulated GPP to the ecophysiological parameters and the effective soil rooting depth. They treated soil rooting depth as a parameter. For VBSA, they identified the uncertainty in each ecophysiological parameter and the soil depth in the form of pdfs. They found that GPP is mainly sensitive to 5 ecophysiological parameters and the soil rooting depth, while others were found to have negligible influence on simulated GPP. In this study, we included these 6 input parameters (highlighted in Table 1) for calibration, whose prior pdfs were assumed identical to that identified by Raj et al. (2014). Other input parameters were fixed at the mean value of the distribution provided by Raj et al. (2014).

[Table 1 about here.]

3.3.2 The likelihood

Recall from Section 3.2.1 that the likelihood is determined by the pdf of the residuals, $e_t = z_t - y_t$ (Eq. 2). Hence, the likelihood function evaluates how well the BIOME-BGC simulated GPP, $\mathbf{y}$, is able to reproduce the data, $\mathbf{z}$. The likelihood function typically defined assuming that the residuals are independent and identically normally distributed (Starrfelt and Kaste, 2014; Braakhekke et al., 2013; Reinds et al., 2008; Svensson et al., 2008; van Oijen et al., 2005). This assumes that the simulator

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models perfectly the temporal profile of GPP leaving no residual temporal correlation in the residuals from the time series. This assumption may not be correct.

BIOME-BGC simulates the time series of GPP at daily time steps. We relaxed the assumption that the temporal profile of simulated GPP perfectly follows the flux tower GPP and modelled the temporal correlation in the residuals. We adopted a likelihood that assumes the residuals follow an autoregressive process of order one (Vrugt, 2016), given as:

$$p_{\log}(\mathbf{z}|\boldsymbol{\theta}) = -\frac{n}{2}\log(2\pi) + \frac{1}{2}\log\left(1-\phi^2\right) - \frac{1}{2}\left(1-\phi^2\right)\hat{\sigma}_1^{-2}e_1^2 - \sum_{t=2}^{n}\log(\hat{\sigma}_t) - \frac{1}{2}\sum_{t=2}^{n}\left(\frac{e_t-\phi e_{t-1}}{\hat{\sigma}_t}\right)^2 \quad (5)$$

where ϕ and $\hat{\sigma}$ are nuisance parameters that are inferred jointly with $\boldsymbol{\theta}$. The parameter $|\phi| < 1$ accounts for the temporal correlation in the residuals, $\mathbf{e}$ and $\phi = 0$ means that there is no temporal correlation. We evaluated whether the posterior distribution ϕ were different from zero (Section 4.1).

Equation 5 gives the likelihood on the logarithmic scale. This improves numerical stability by avoiding rounding errors in the computation. n is the length of the vectors $\mathbf{z}$ and $\mathbf{y}$.

3.3.3 Posterior prediction of BIOME-BGC parameters and GPP

We implemented DREAM algorithm in MATLAB version R2015b. The DREAM toolbox was provided by its developer, Jasper A. Vrugt, from University of California, Davis, USA. Technical details of the DREAM toolbox are provided by Vrugt (2016).

We used $N = 10$ Markov chains with $T = 15000$ iterations for each chain. This produced 150000 ($N \times T$) posterior samples for each θ_j ($j = 1, 2, .., 6$ for selected BIOME-BGC parameters for calibration). Gelman et al. (2013) and Vrugt et al. (2009) recommend discarding the first 50% of the samples as a burn-in; however, we discarded 10000 samples, in order to reduce the computation cost. This resulted in 50000 ($N \times (T - \text{burn-in})$) post burn-in samples for each θ_j. The convergence of these post burn-in samples was evaluated using the Gelman–Rubin diagnostic (Gelman and Rubin, 1992) and through visual examination of the trace plots. The Gelman–Rubin potential scale reduction factor (PSRF) compares the between-chain and within-chain variance of the parallel Markov chains. A PSRF close to 1 indicates that the chains have converged.

The post burn-in samples created 50000 vectors of $\boldsymbol{\theta}$. BIOME-BGC was run at each parameter vector using daily meteorological data of 2009 and the daily simulated GPP (posterior prediction of GPP) was evaluated and stored. This produced the distribution of daily GPP, which was summarized by the median and the 2.5 and 97.5 percentile (i.e., 95 % credible interval). The 95 % credible interval showed the uncertainty in the daily simulated GPP. We compared these 95 % credible intervals and medians over the growing season with that of flux tower GPP.

We conducted two experiments to obtain the posterior samples of $\boldsymbol{\theta}$:

1. Experiment 1: We used daily flux tower GPP for five months in the growing season (April to August 2009) to calibrate BIOME-BGC for the growing season. For calculation of the log-likelihood using Eq. (5), we set $n = 153$, equal to the

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number of days in April to August. Note that we did not include the daily flux tower GPP for September and October in the calibration and we used these data for validation of the calibrated BIOME-BGC. In this experiment, the obtained posterior samples of $\boldsymbol{\theta}$ were used to simulate GPP and the associated uncertainty for each day in 2009.

2. Experiment 2: We used daily flux tower GPP for one month only, e.g., April, in the growing season to calibrate BIOME-BGC. For the likelihood calculation, we set $n = 30$, equal to the number of days in April. The obtained posterior distributions of $\boldsymbol{\theta}$ were used to simulate daily GPP with the associated uncertainty for 2009. We then extracted the daily simulated GPP (with the associated uncertainty) of April only and discarded the other months in 2009. Likewise, we obtained the simulated GPP and the associated uncertainty for the other six months (May to October 2009) in the growing season. Experiment 2 resulted in seven different posterior samples of $\boldsymbol{\theta}$.

For both experiments, we followed the same procedure explained in the paragraph 2 and 3 of this section.

3.3.4 Statistical evaluation of BIOME-BGC simulated GPP

We determined the performance of the calibration using two criteria that evaluate efficiency with which the calibrated BIOME-BGC reproduces the flux tower GPP. Both criteria provide a single measure of BIOME-BGC efficiency in simulating daily GPP over the selected period. The first criterion was the root mean square error (RMSE) between the simulated and flux tower GPP:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{t=1}^{n}(z_t - y_t)^2} \tag{6}$$

where n is the number of daily flux tower GPP (z_t) and the simulated GPP (y_t). RMSE has the units of GPP. A low value of RMSE indicates the high accuracy. The second criterion was the Nash-Sutcliffe efficiency (NSE) (Nash and Sutcliffe, 1970):

$$\mathrm{NSE} = 1 - \frac{\sum_{t=1}^{n}(z_t - y_t)^2}{\sum_{t=1}^{n}(z_t - \overline{z})^2} \tag{7}$$

where $\overline{z}$ is the mean of the observations (flux tower GPP). NSE can range from $-\infty$ to 1. An NSE value close to 1 indicates high accuracy in the simulation of GPP. Following Dumont et al. (2014), we assumed that a NSE ≥ 0.5 indicates adequate accuracy in the simulated GPP.

We evaluated the performance of BIOME-BGC for the following cases:

1. For Experiment 1, we obtained RMSE and NSE for the two periods: calibration period of five months (April to August) and the validation period of two months (September and October). For each period, the calculations were made for 2.5 percentiles, 97.5 percentiles, and medians. Note that the RMSE and NSE are typically evaluated at the median of the posterior predictive distribution; however, this does not evaluate the posterior uncertainty (Hamm et al., 2015a). Therefore we also calculated the RMSE and NSE for the 2.5 and 97.5 percentiles of the posterior predictive distribution of BIOME-BGC simulated GPP ($y_{2.5}$ and $y_{97.5}$) against the same percentiles for the posterior predictive distribution of flux tower GPP ($z_{2.5}$ and $z_{97.5}$).

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2. For Experiment 2, we obtained RMSE and NSE for the same two periods and percentiles as stated in point 1 (above), to make a direct comparison with the results of Experiment 1.

3. To show the performance of uncalibrated BIOME-BGC, we obtained the daily simulated GPP with 95% credible intervals at the prior distributions of six selected parameters (Table 1). We sampled from these prior distributions to obtain 50000 parameter vectors. BIOME-BGC was run at these parameter vectors to yield the prior predictor of BIOME-BGC simulated GPP. We calculated the RMSE and NSE for the same two periods and percentiles as stated in point 1, to make a direct comparison with Experiments 1 and 2.

4 Results

4.1 Convergence of the Markov chains

The value of Gelman–Rubin PSRF was close to one for each θ_j obtained in both experiments (Table 2). Figures 1a to 1f show the trace plots of each θ_j for Experiment 1. Visual inspection of the trace plots indicated that all ten Markov chains were mixed properly with each other. For Experiment 2, we also observed the convergence of the Markov chains for each θ_j in each month of the growing season (trace plots not shown here). The visual and statistical diagnostic demonstrated that each θ_j had explored its range and the obtained samples from the converged chains were the samples from the posterior distribution.

Figure 1g shows the trace plot of ϕ, accounting for the temporal correlation in the error residuals (section 3.3.2), for Experiment 1. We observed $\phi \neq 0$ and its value ranged from 0.56 to 0.93 with a mean at 0.75. The non-zero values of ϕ indicated that the residuals are temporarily correlated, thus supporting our choice of likelihood function (Eq. 5). For Experiment 2, non-zero values of ϕ were also obtained in each month.

[Figure 1 about here.]

[Table 2 about here.]

4.2 Posterior distribution of BIOME-BGC parameters

Figure 2 shows the temporal profile of median and 95% credible interval of each θ_j over the growing season for Experiment 2. The median and 95 % interval for Experiment 1 is constant, since this did not vary over time. For both experiments, we observed that the uncertainty in the posterior distribution of each θ_j was reduced compared to the prior distribution, indicating that $\boldsymbol{\theta}$ were constrained by the flux tower GPP observations. These uncertainties were higher in Experiment 2 than that of Experiment 1. The upper quantiles (97.5%) of the posterior distributions of the parameters LFRT, FRC:LC, and SD were found close to the maximum values of the corresponding prior distributions for both experiments. The uniform priors of these parameters (Table 1) possibly imposed an upper boundary in the posteriors. We chose to keep these maximum values since the choices, given in Table 1, were based on the realistic ranges of LFRT, FRC:LC, and SD for Dougls-fir at Speulderbos.

For Experiment 2, the uncertainties in LFRT, FRC:LC, W_{int}, and SD were higher at the start and end of the growing season compared to other months. The uncertainties in these parameters were lowest during the peak of the growing season (July and

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August). The values of LFRT, FRC:LC, and SD increased during the peak of the growing season and became close to that obtained in Experiment 1 and then started decreasing. The opposite trend was observed for W_{int}. The uncertainty in C:N_{leaf} for any month obtained in Experiment 2 was comparable and within the range of that obtained in experiment 1. We did not find significant variation in the trend of FLNR obtained in Experiment 2 during the growing season; however, higher uncertainty in FLNR was observed compared to Experiment 1.

[Figure 2 about here.]

4.3 Evaluation of calibrated BIOME-BGC for Experiment 1

We evaluated the performance of calibrated BIOME-BGC by comparing the daily simulated posterior GPP and the daily posterior flux tower GPP, for the calibration period of April to August (Fig. 3) and the validation period of September and October (Fig. 4). The daily simulated and flux tower GPP were summarized by the median and 95% credible interval. The temporal profile of these medians and credible intervals were plotted against that of flux tower GPP. Evaluation of the BIOME-BGC before and after calibration (Experiment 1) based on the statistical criteria (RMSE and NSE) is shown in Table 3. The periods for which these criteria were obtained are explained in Section 3.3.4.

Overall, posterior predicted daily GPP was close to flux tower GPP during the calibration period (Fig. 3), although the separation between these two temporal profiles in April (Julian day 91 to 120) was large compared to other months (Julian day 121 to 242) in the growing season. For the validation period, the simulated GPP closely followed the flux tower GPP (Fig. 4).

The posterior predicted BIOME-BGC GPP was improved compared with the prior predicted BIOME-BGC, as indicated by the drop of RMSE for the median as well as the 2.5 and 97.5 percentil0e for both calibration and validation periods (Table 3). The NSE criterion was also improved after calibration (NSE > 0.5), whereas before calibration, the value of NSE was negative. The enhancement in NSE and the drop of RMSE give statistical evidence of the improvement in the daily simulated GPP after calibration.

[Figure 3 about here.]

[Figure 4 about here.]

[Table 3 about here.]

4.4 Relation of posterior simulated GPP with meteorological variables

Most of the variability of daily BIOME-BGC output was due to the meteorological input data. Figure 5 illustrates this by showing the seasonal variation of the medians of the daily posterior predicted GPP, obtained from Experiment 1, together with Tday, VPD, srad, and precipitation. Tday, VPD, and srad were correlated strongly with each other and the posterior predicted GPP followed the pattern of these input variables. In general between days, we observed that the increase in Tday, VPD, and srad increased GPP and vice-versa. The daily simulated GPP had a strong positive correlation with Tday, with a correlation coefficient $r = 0.85$. GPP showed less positive correlation with VPD and srad, compared to Tday, with $r = 0.71$ and $r = 0.66$

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respectively. A negative, but weak (> -0.5), correlation was found between GPP and precipitation with $r = -0.22$. This is due to the negative correlation that rainfall has with srad, VPD and Tday, whereas the effect on GPP is usually not immediate due to the replenishment of the soil water reservoir.

Because BIOME-BGC simulates the seasonal phenology, the daily simulated GPP on a particular Julian day is not temporarily independent. GPP depends on the history of the meteorological data. To verify this, we swapped the meteorological data of Julian days 91-166 with those of days 167-242, ran BIOME-BGC with the swapped meteorological data with the posterior samples of $\boldsymbol{\theta}$ (obtained from Experiment 1) and then reversed the generated output of GPP back into the original order. Figure 6 compares the temporal profile of the medians of GPP_{sp} (GPP swapped) with those obtained from Eperiment 1 (section 4.3) with the meteorological data in the correct order. If only the meteorological data of a particular day and the input parameters would be responsible for daily simulation, the temporal profile of GPP_{sp} and GPP_{exp1} should have matched exactly; however, this is not the case. We observed a difference in daily GPP_{sp} and GPP_{exp1}. The swapping of meteorological data led to an over- and underestimation of daily GPP_{sp} with a maximum of 1.4 and 1.8 gC m^{-2} s^{-1} respectively. This indicated clearly that the daily simulated GPP was temporarily dependent and did not depend only on the meteorological data and the input parameters for a given day. This temporal dependency was due to the update of the BIOME-BGC storage terms between days.

[Figure 5 about here.]

[Figure 6 about here.]

4.5 Posterior simulated GPP for Experiment 2

Combining the daily simulations of each month provided the temporal profile of the medians and 95% credible intervals of the daily simulated posterior GPP over the growing season. Figure 7 shows this temporal profile (black line and grey shade) from April to August. We observed that the posterior predicted GPP had a better fit to the flux tower GPP, compared to Experiment 1 (Fig. 3). Particularly, the posterior predicted GPP of April (Julian days 91 to 120) followed the flux tower GPP more closely than Experiment 1. We found further enhancement in the NSE compared to Experiment 1 for the median, 2.5, and 9.5 percentile over the period of April to August (Table 3) where the values of NSE became closer to 1. A drop in RMSE was also observed. For the period of September and October (temporal profile not shown here), however, the NSE and RMSE were the same as for Experiment 1. These results indicated an improvement in the posterior predicted GPP compared to that obtained from Experiment 1, but at the expense of a higher degree of freedom.

[Figure 7 about here.]

5 Discussion

5.1 Simulatoin of GPP using BIOME-BGC

To explain our results, we identified the processes within BIOME-BGC that are controlled by the six calibrated parameters and relate to the simulation of GPP (Fig. 8). These processes are implemented by different routines. The routines, however, are

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controlled not only by these six parameters, but also generate intermediate outputs, as shown in Fig. 8. We only highlight those routines that were relevant to the simulation of GPP. We refer the reader to Thornton (2010) for a detailed explanation of the routines.

BIOME-BGC simulates the daily development of plant carbon pools (White et al., 2000). The development of carbon pools is governed by the daily update of BIOME-BGC memory of mass of carbon stored in different components of the plant. The simulated development of plant carbon pools on a particular day is dependent on the previous days. BIOME-BGC converts the carbon stored in the leaf pool (leaf C) into an equivalent leaf area index (LAI). The development of leaf C controls the development of LAI in the radiation transfer routine. Leaf C relates to the loss of leaf biomass, which is expressed as the parameter LFRT. The parameter FRC:LC is also responsible for the development of leaf C and then LAI. In the precipitation routine, W_{int}, together with LAI, determines the amount of precipitation intercepted by the canopy, which in turns controls the amount of water that reaches the soil. The soil psi routine calculates the volumetric water content in the soil as the ratio of soil water to SD. Thereafter, soil water potential is derived as a function of volumetric water content. The soil water potential acts as a multiplier in the evapotranspiration routine to simulate stomatal closure and the leaf scale conductance to water vapour per unit leaf area.

The photosynthesis routine converts the conductance to water vapour to the conductance for CO_2, which measures the rate of passage of CO_2 into the leaf stomata. The parameter C:N_{leaf} together with LAI determines the leaf nitrogen content from the carbon pool in the photosynthesis routine and the day leaf maintenance respiration per unit leaf area in the respiration routine. The leaf scale conductance to CO_2, leaf nitrogen content, day leaf maintenance respiration and the parameter FLNR are further used in the Farquhar model, implemented in the photosynthesis routine, to simulate the carboxylation capacity (V_{cmax}) and thus the carbon assimilation. The assimilated carbon is then added to the day leaf maintenance respiration and then multiplied by the LAI and daylength to simulate the daily GPP. The respiration routine also calculates the maintenance respiration of root and stem (not shown in Fig. 8) together with leaf. The respiration terms are summed and then subtracted from GPP to obtain available carbon for allocation, which further updates leaf C. Finally, Fig. 8 indicates which meteorological variables are used in a given routine, although we have not described their specific role.

We presented the link between six calibrated parameters and the BIOME-BGC internal routines so that we could explain our results considering the development of the state variables, principally such as LAI and V_{cmax}. LAI and V_{cmax} exhibit a seasonal cycle and affect the seasonality of simulated GPP. This is explored further in Section 5.2.

[Figure 8 about here.]

5.2 BIOME-BGC calibration

BIOME-BGC accounts for dynamic for carbon stocks in the vegetation by means of allocation, hence it uses parameters that are constant for the year of simulation. Consider Experiment 1. The memory of BIOME-BGC is updated between days (Section 5.1), and Biome-BGC takes care of the simulation of time-varying state variables such as leaf area index (LAI) and carboxylation capacity (V_{cmax}) used in Farquhar's model. Therefore, the daily simulated GPP are temporarily dependent, which was highlighted experimentally in our study by the swapping of meteorological variables between Julian days 91-166

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and 167-242 (Fig. 6). The posterior predicted GPP closely followed the posterior predicted flux tower GPP even for those months (September and October) which were not included in the calibration (Fig. 4), although this was not perfect as shown by the fact that $\phi \neq 0$. If the simulator would properly capture the temporal development of GPP we would expect that $\phi = 0$, even after allowing for some uncertainty in the prediction. The fact that the residuals showed temporal autocorrelation indicated that the representation of dynamic processes within the simulator could be improved.

Experiment 1 showed that BIOME-BGC was able to reproduce closely the posterior predicted flux tower GPP. Further, the Bayesian calibration allowed daily GPP simulation as well as quantification of the associated uncertainty (Figs. 3 and 4). Furthermore, the apparent overprediction of daily simulated GPP, compared to flux tower GPP, for the month of April raised questions: (a) on the reliability of simulated GPP for those months that were not included in this study; and (b) whether the seasonal cycle of all of the state variables was simulated realistically. These questions led us to estimate the time varying posterior distributions of parameters in Experiment 2. We recognize that this contradicts the specified use of BIOME-BGC since it (a) violates the requirement of constant parameters and (b) affects the update of the state variables over time. Nevertheless, the experiment did allow more flexibility to vary the parameters over time, with consequences for the update of state variables and the posterior prediction of GPP.

Consider Experiment 2. Note that BIOME-BGC actually simulated daily GPP for a whole year with the posterior distributions of the parameters of each month. We selected only the daily simulated GPP of that month to which the posterior distributions belong and we discarded other eleven months of simulations. The temporal profile in Fig. 7 is the combinations of daily simulated GPP of each month in the growing season (Section 3.3.3 and 4.5). We observed an improvement (Fig. 7), particularly in the month of April, in the daily posterior predicted GPP compared to Experiment 1 (Fig. 3). This improvement was also clear in Table 3 which shows an increase in the NSE and decrease in the RMSE for Experiment 2 compared to Experiment 1. The calibration approach adopted in Experiment 2 was more flexible and led to increased prediction accuracy despite contradicting the BIOME-BGC design.

Experiment 2 showed variation in the six calibrated parameter over the growing season (Fig. 2), particularly W_{int}, SD , FRC:LC, and LFRT. These variations were also in-line with the seasonal variation in GPP. For example, maintaining the high GPP rates during the peak of the growing season (July and August), required more soil water, which was obtained by decreasing the parameters W_{int}, in turn affecting the water intercepted by the canopy (precipitation routing routine in Fig. 8), and increasing the soil rooting depth (SD). The parameters FRC:LC and LFRT also increased and both affected GPP through LAI. The variation in FLNR and C:N_{leaf}, which together determined V_{cmax}, also changed month-by-month (Fig. 8). These results indicated that Biome-BGC, with the six parameters that we calibrated, may be able to accurately simulate the seasonal cycle of some state variables, but may be too rigid to simulate all state updates. The result was that the posterior predictive distribution of the parameters varied month-by-month with consequences for the posterior predicted BIOME-BGC GPP. Specifically the predictions improved (lower RMSE, higher NSE) relative to Experiment 1. To our knowledge, this aspect has not been discussed in earlier work on the calibration of BIOME-BGC (Yan et al., 2014; Ueyama et al., 2010; Maselli et al., 2008).

In this study we performed our calibration based on six parameters (LFRT, FRC:LC, C:N_{leaf}, W_{int}, FLNR, and SD) whereas BIOME-BGC has 35 parameters in total. A calibration based on 35 parameters was not feasible computationally so, in line with

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other authors (e.g., Minunno et al., 2013), we chose a subset of the parameters. We defend our choice of parameters based on our previous experimental results, which showed that annual total GPP was most sensitive to these parameters (Raj et al., 2014) at Speulderbos. Nevertheless, GPP may be sensitive to other parameters at finer spatial scales. Computational developments and the flexibility of the DREAM algorithm may allow more parameters to be calibrated, so this should be explored further in future.

6 Conclusions

This study presented a calibration of BIOME-BGC. We illustrated the framework at the Speulderbos forest site, the Netherlands. Our study led to the following conclusions:

1. Quantification of uncertainty in the simulated GPP is not integrated into BIOME-BGC, although Monte Carlo approaches allow exploration of uncertainty due to uncertain parameters. The Bayesian framework allowed quantification of uncertainty in both the estimated parameters and the predicted GPP, through the posterior (predictive) distribution. The uncertainty is important in the sense that it helps to determine how much confidence can be placed in the results of forest carbon related studies based on GPP. A calibration based on optimization of BIOME-BGC parameters, as done in earlier studies, can not capture the associated uncertainty in the simulated GPP.

2. We modelled the temporal correlation in the residuals through the nuisance parameter, ϕ, in the likelihood function. Our results supported the use of temporal correlation in the residuals for the inference of the posterior parameter distributions of BIOME-BGC. This showed that BIOME-BGC did not properly simulate the temporal profile of GPP. Hence the calibration also gave greater insight into the simulator. Future research should identify the cause of this limitation.

3. We used the calibration results to gain further insights into the functioning of BIOME-BGC through analysis of the time varying posterior parameter distributions. Our study revealed that the constant distributions of BIOME-BGC parameters were not adequate to simulate the seasonality in daily GPP. The seasonality was captured more precisely by using time varying parameters. This reinforces our previous conclusion. The implications of temporal correlation and time-varying parameters should receive attention from the BIOME-BGC modelling community.

4. We implemented our calibration using the DREAM algorithm and its freely available MATLAB toolbox. DREAM offers considerable computational advantages and flexibility compared to other MCMC implementations and is gaining increased usage. It shows promise for biogeochemical and other environmental simulation applications. Specifically future research could calibrate more parameters.

7 Code and data availability

We provide a MATLAB script and input data as a supplementary material to support the implementation of Bayesian calibration of the BIOME-BGC simulator. The MATLAB script uses the functionality of the DREAM toolbox, which can be obtained,

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on request, from its developer Jasper A. Vrugt, University of California, Davis, USA (Vrugt, 2016). The source code of the BIOME-BGC simulator can be downloaded from http://www.ntsg.umt.edu/project/biome-bgc. Markov chains in DREAM are run in parallel using multiple cores of the computer processors. DREAM consumes a large amount of memory (RAM). The experiment shown in this manuscript was performed on Windows Server 2012 Dell Precision 7910 with a twelve-core Xeon processor and 128 GB of RAM.

The description of each file in the supplementary material is given below:

1. MATLAB scripts

   (a) *DREAM_setup.m*: This scripts defines the basic settings of DREAM, which were used in our experiment. The script is self explanatory. This script calls the MATLAB function ("BIOME-BGCrunScript.m") to run BIOME-BGC simulator.

   (b) *BIOME-BGCrunScript.m*: This scripts defines the function to run BIOME-BGC (by calling pointbgc.exe) simulator with the parameters value obtained in each iteration of DREAM and the daily simulated GPP (gross primary production) is returned. We do not provide "pointbgc.exe". This can be obtained by compiling BIOME-BGC source code.

2. Input data files used to run BIOME-BGC in our experiment (For details, see BIOME-BGC user guide that comes with the source code of BIOME-BGC)

   (a) *enf_speuld_Main.ini*: This is the input initialization file. It provides general information about the simulation such as site characteristic data, the name of all required input files and output files, and lists of output variables to be stored.

   (b) *Meanpm.epc*: This is the input parameters file that contains mean value of each parameter.

   (c) *Speuld2009.mtc41*: This file contains daily input meteorological variables of 2009 at Speulderbos site, the Netherlands.

3. Input flux tower GPP (for calibration and comparison with posterior simulated GPP)

   (a) *Percentiles_FluxTower_GPP_JD_91_304.xlsx*: This excel file contains mean and percentiles of daily GPP (for the growing season of 2009) partitioned from flux tower measurements of net ecosystem exchange at the Speulderbos forest site, the Netherlands. Daily mean values were used in calibration and percentiles values were used to compare with posterior simulated GPP.

   (b) *TowerGPP.txt*: This file contains the subset (from Julian day 91 to 243 in Experiment 1, see Section 3.3.3) of daily mean of flux tower GPP. This file is called in "DREAM_setup.m". For Experiment 2, different subsets of flux tower GPP can be easily obtained from the file "Percentiles_FluxTower_GPP_JD_91_304.xlsx".

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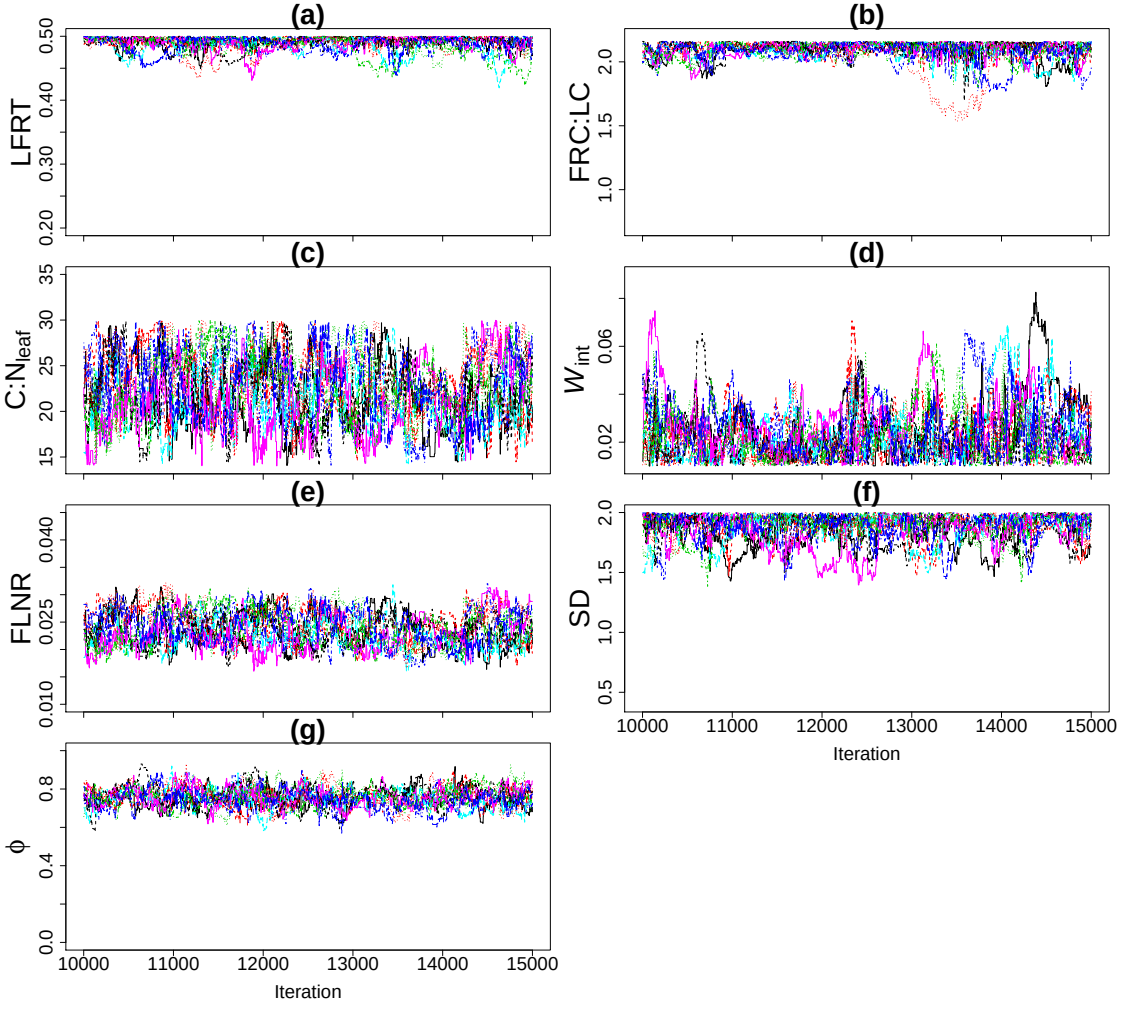

Figure 1. Trace plot of each calibrated BIOME-BGC parameter and ϕ for Experiment 1. Information about the BIOME-BGC parameters is given in Table 1.

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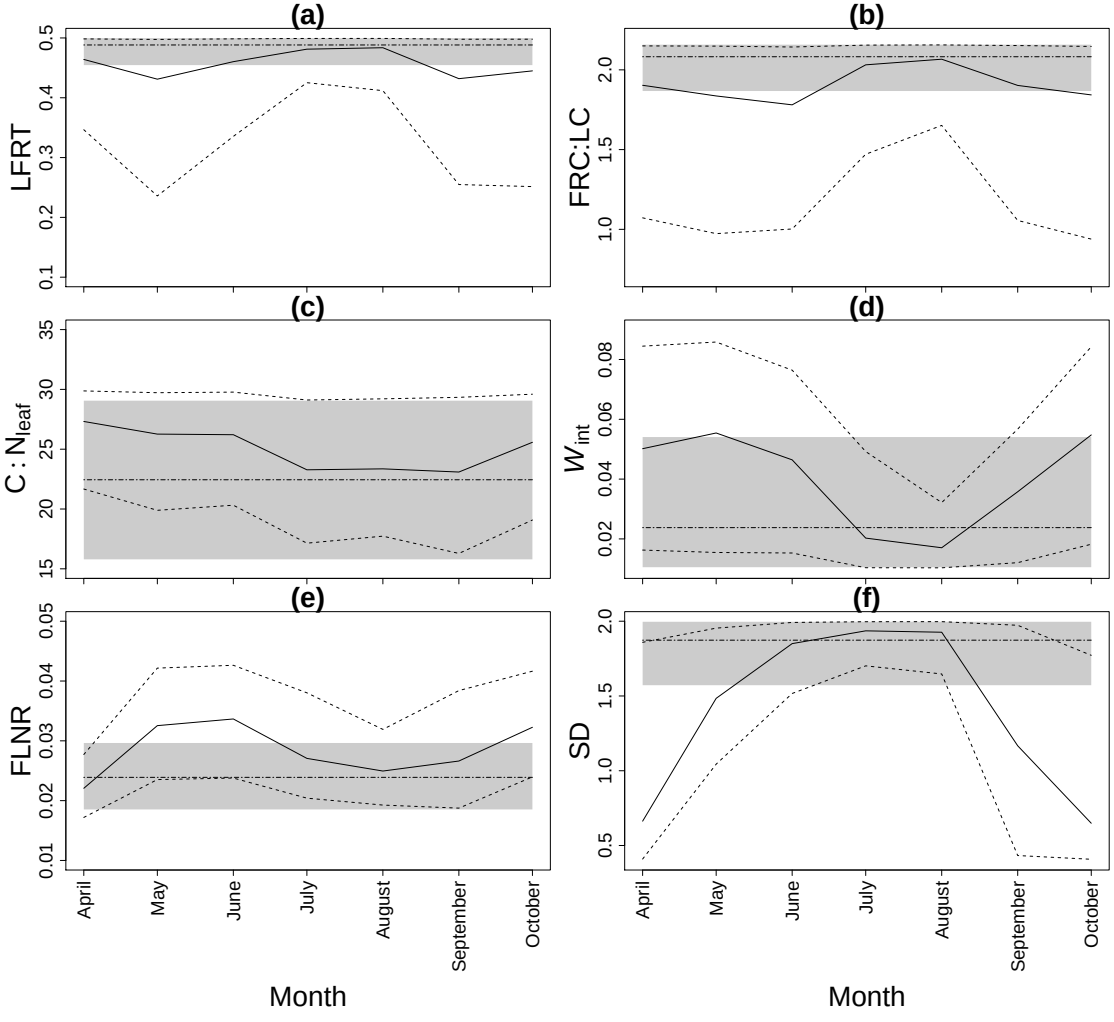

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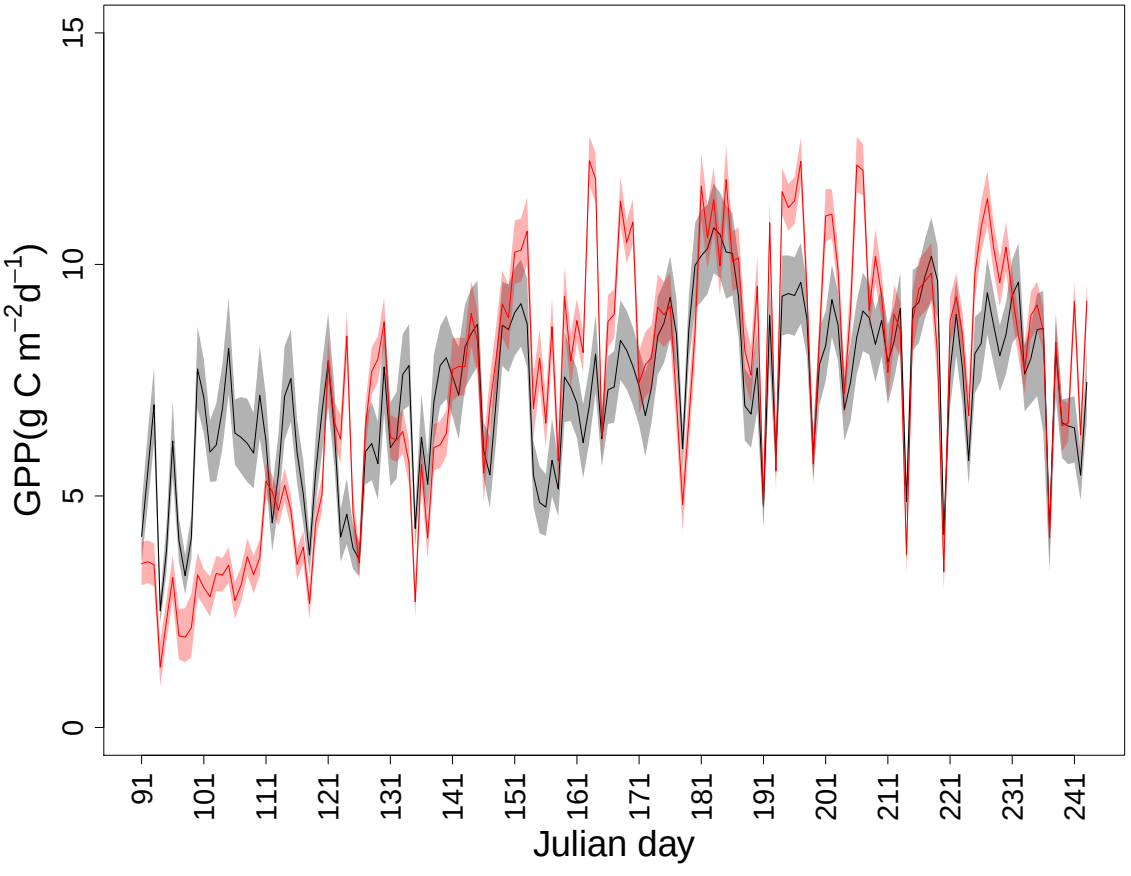

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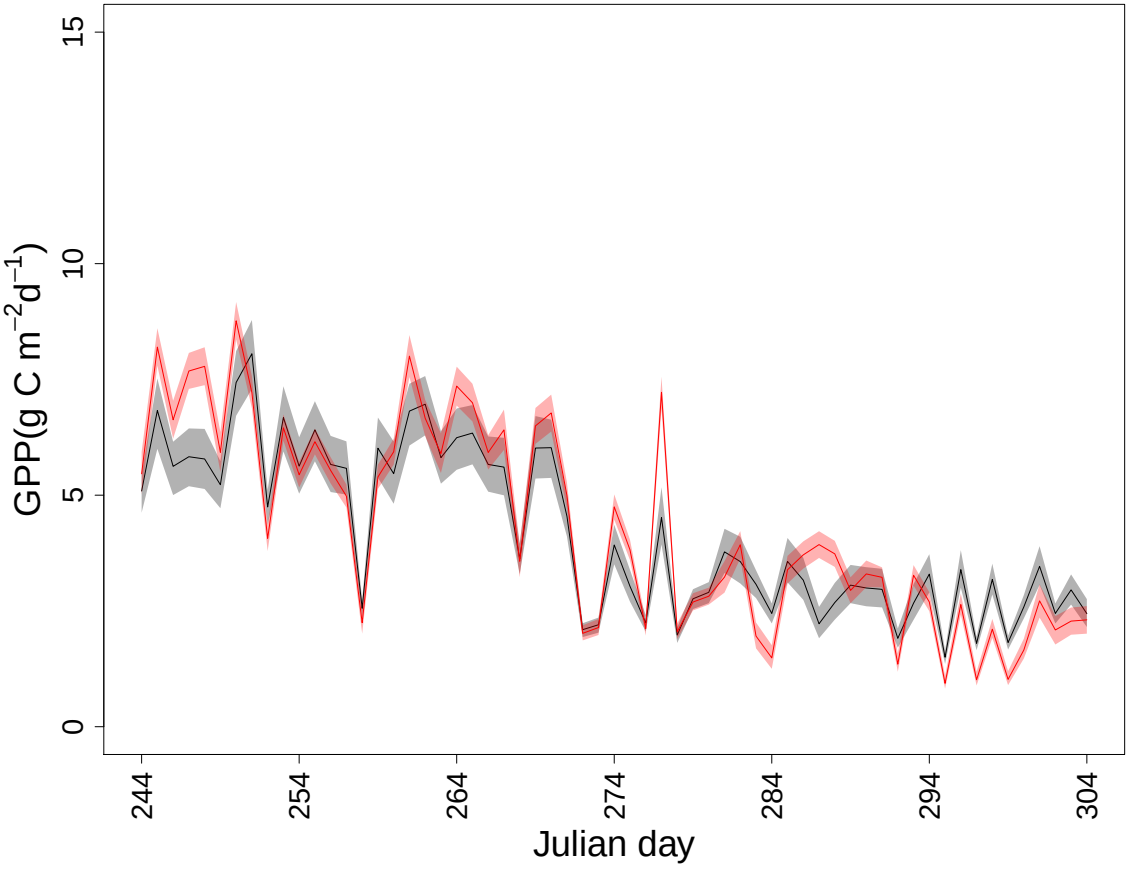

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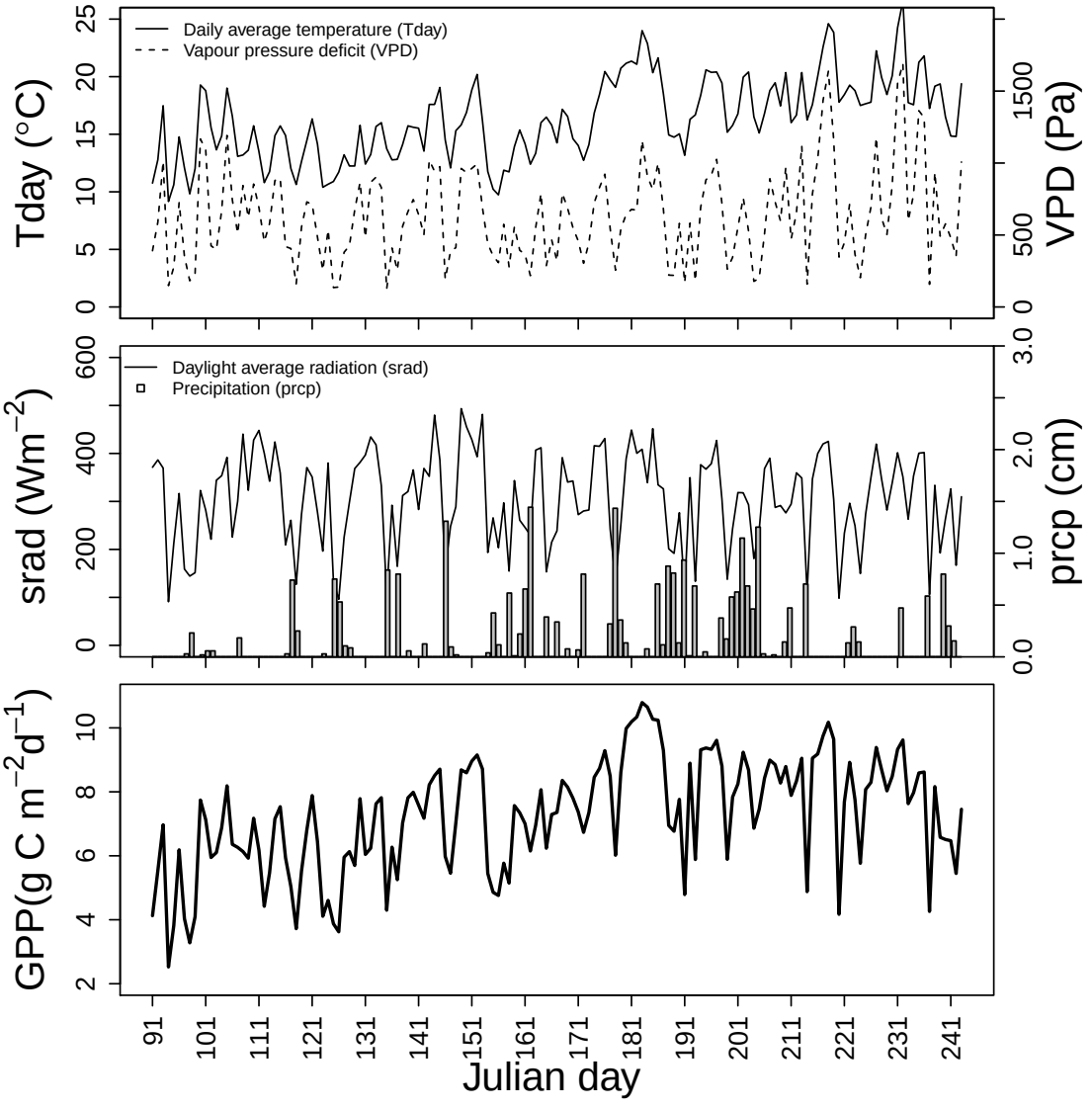

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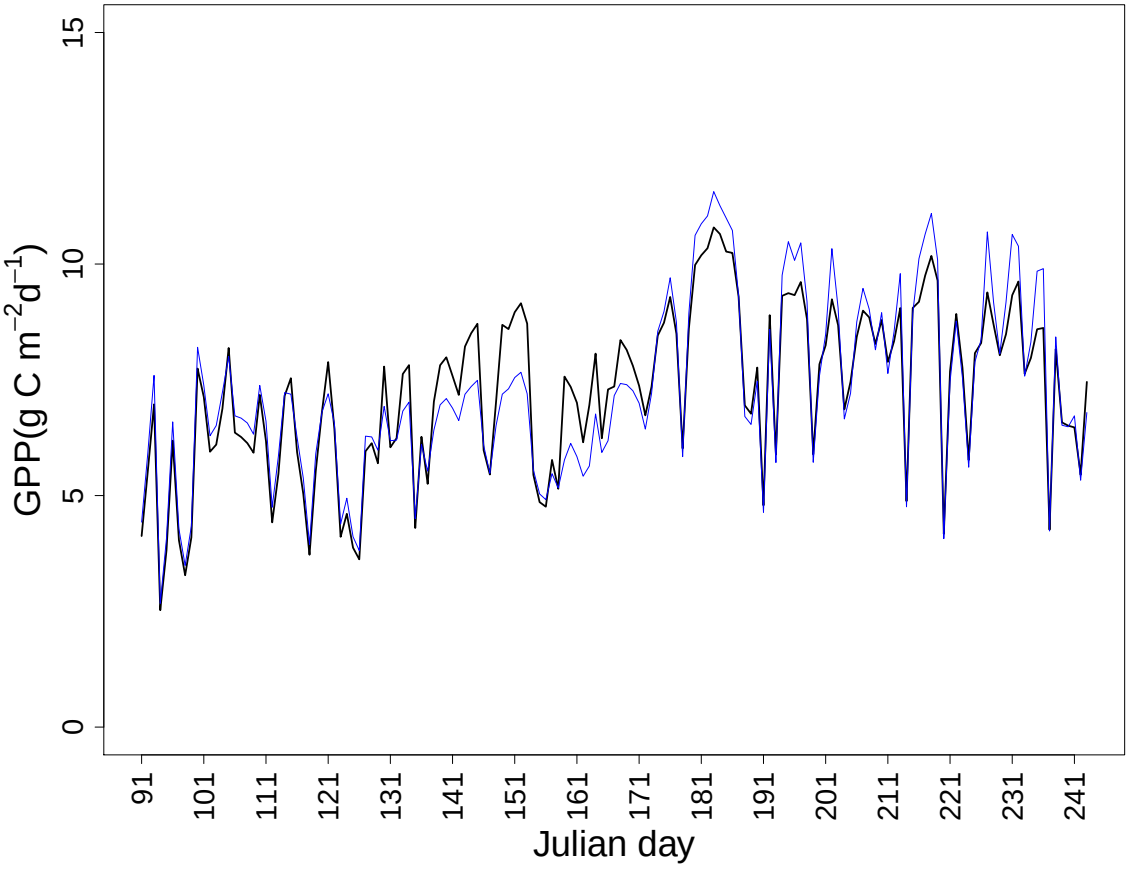

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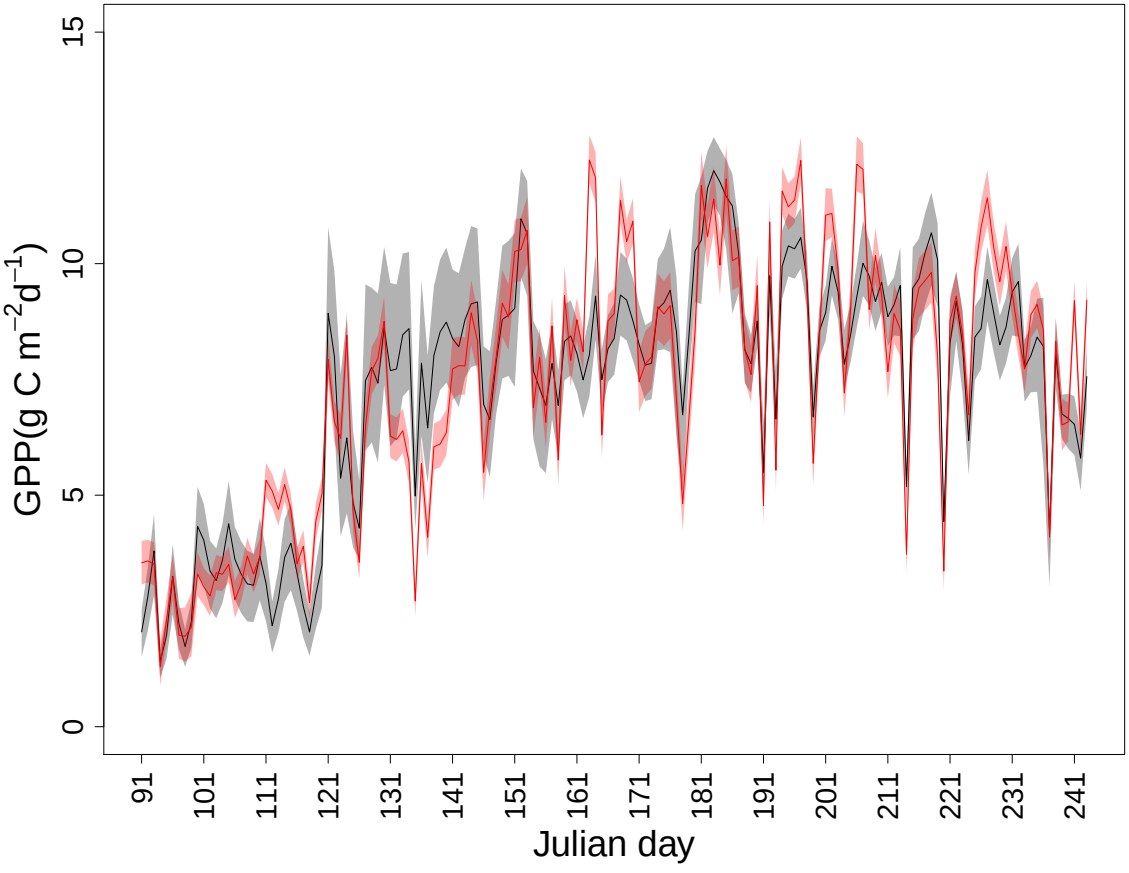

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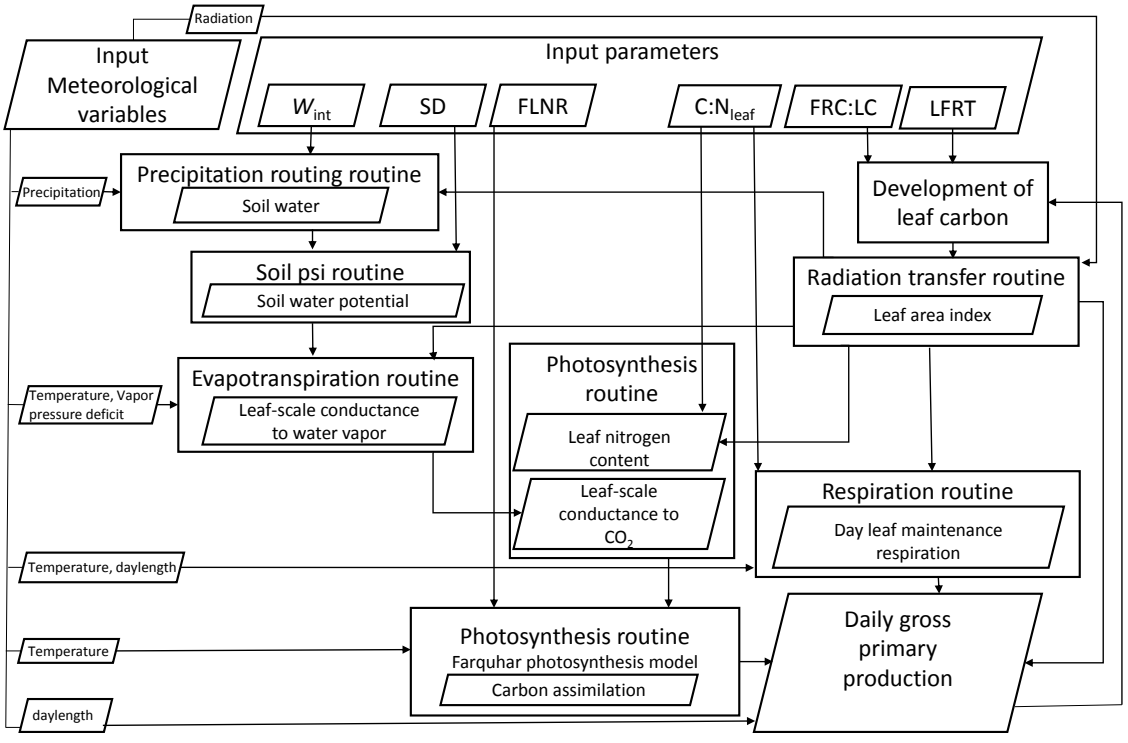

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Ecophysiological parameter	Symbol	Unit	Mean value/distribution[†]
Leaf and fine root turnover	**LFRT**	1 yr^{-1}	$U(0.196, 0.5)^{\dagger}$
Annual live wood turnover fraction	LWT	1 yr^{-1}	0.70
Annual whole-plant mortality fraction	WPM	1 yr^{-1}	0.005
Annual fire mortality fraction	FM	1 yr^{-1}	0.005
new fine root C : new leaf C	**FRC:LC**	kg C (kg C)$^{-1}$	$U(0.78, 2.16)^{\dagger}$
new stem C : new leaf C	SC:LC	kg C (kg C)$^{-1}$	2.391
new live wood C : new total wood C	LWC:TWC	kg C (kg C)$^{-1}$	0.071
new croot C : new stem C	CRC:SC	kg C (kg C)$^{-1}$	0.262
Current growth proportion	CGP	Prop.	0.5
C:N of leaves	**C:N_{leaf}**	kg C (kg N)$^{-1}$	$\mathcal{N}(26.731, 3.731)^{\dagger}$
C:N of leaf litter, after retranslocation	C:N_{lit}	kg C (kg N)$^{-1}$	31.625
C:N of fine roots	C:N_{fr}	kg C (kg N)$^{-1}$	54.8
C:N of live wood	C:N_{lw}	kg C (kg N)$^{-1}$	54.8
C:N of dead wood	C:N_{dw}	kg C (kg N)$^{-1}$	1029.5
Leaf litter labile proportion	L_{lab}	Unitless	0.644
Leaf litter cellulose proportion	L_{cel}	Unitless	0.201
Leaf litter lignin proportion	L_{lig}	Unitless	0.155
Fine root labile proportion	FR_{lab}	Unitless	0.527
Fine root cellulose proportion	FR_{cel}	Unitless	0.378
Fine root lignin proportion	FR_{lig}	Unitless	0.095
Dead wood cellulose proportion	DW_{cel}	Unitless	0.772
Dead wood lignin proportion	DW_{lig}	Unitless	0.228
Canopy water interception coefficient	$\boldsymbol{W_{int}}$	1 LAI^{-1} day^{-1}	$\mathcal{N}(0.04, 0.02)^{\dagger}$
Canopy light extinction coefficient	k	Unitless	0.453
All-sided to projected leaf area ratio	$LAI_{all:proj}$	LAI LAI^{-1}	2.572
Canopy average specific leaf area	SLA	m^2 (kg C)$^{-1}$	14.65
Ratio of shaded SLA:sunlit SLA	$SLA_{shd:sun}$	SLA SLA^{-1}	2.0
Fraction of leaf N in Rubisco	**FLNR**	Unitless	$B(25.67, 756.28)^{\dagger}$
Maximum stomatal conductance	g_{smax}	m s^{-1}	0.0051
Cuticular conductance	g_{cut}	m s^{-1}	0.000051
Boundary layer conductance	g_{bl}	m s^{-1}	0.075
Leaf water potential: start of conductance reduction	LWP_i	Mpa	-0.647
Leaf water potential: complete conductance reduction	LWP_f	Mpa	-2.487
Vapor pressure deficit: start of conductance reduction	VPD_i	Pa	610.0
Vapor pressure deficit: complete conductance reduction	VPD_f	Pa	3130.0
Site characteristic			
Effective soil Depth	**SD**	meter	$U(0.4, 2)^{\dagger}$

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Table 2. Gelman–Rubin potential scale reduction factor (PSRF) of each BIOME-BGC parameter selected for calibration and ϕ for experiment 1 and 2.

	PSRF							
	Experiment 1	Experiment 2						
Parameter ↓ \ Julian days →	91-243	91-120	121-151	152-181	182-212	213-243	244-273	274-304
LFRT	1.05	1.03	1.01	1.03	1.03	1.04	1.03	1.01
FRC:LC	1.09	1.02	1.01	1.01	1.04	1.06	1.02	1.01
$C:N_{leaf}$	1.04	1.02	1.02	1.01	1.04	1.04	1.03	1.03
W_{int}	1.02	1.01	1.01	1.02	1.06	1.03	1.03	1.01
FLNR	1.04	1.04	1.02	1.01	1.05	1.06	1.02	1.01
SD	1.04	1.03	1.02	1.02	1.03	1.1	1.02	1.02
ϕ	1.02	1.03	1.01	1.01	1.03	1.03	1.01	1.01

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Table 3. Root mean square error (RMSE) and Nash-Sutcliffe efficiency (NSE) between the posterior predicted BIOME-BGC and flux tower GPP for different experiments (see Section 3.3.4).

		2.5%		Median		97.5%	
	Period	RMSE	NSE	RMSE	NSE	RMSE	NSE
Before calibration	April to August	5.06	-2.53	3.74	-0.85	4.26	-1.3
	September-October	2.23	-0.15	1.22	0.68	2.64	-0.42
Experiment 1	April to August	1.84	0.53	1.81	0.57	1.85	0.57
	September-October	0.91	0.81	0.83	0.85	0.79	0.87
Experiment 2	April to August	1.3	0.77	1.24	0.8	1.45	0.73
	September-October	0.94	0.79	0.84	0.85	0.92	0.83