

Date: 07 March 2017

Dear Philippe Peylin,

We are pleased to submit the revised version of our manuscript titled “Bayesian integration of flux tower data into process-based simulator for quantifying uncertainty in simulated output”. We appreciated the constructive criticisms of both referees that have helped to improve the manuscript. The response to the referees is given underneath this letter. We hope that we have addressed the comments to the satisfaction of both referees.

In general we have extended the relevant sections in order to address the referees’ comments. We have referred to these changes in the response to the referees. Unless specifically requested by the referees, we have not substantively altered the content or format of the paper. In the revised manuscript, new text is highlighted in red. Deleted text is indicated by strikethrough. The term “previous manuscript” used below refers to published Geoscientific Model Development discussion paper. The term “revised manuscript” refers to the manuscript attached at the end.

We would like to clarify some points:

1. The most important concerns of both referees are the use of “time varying parameters of BIOME-BGC simulator” and “GPP partitioned from the flux tower measurements of net ecosystem exchange (NEE) in a Bayesian calibration”. We fully understand the concerns of both referees. Regarding time varying parameters (obtained in month wise calibration), we agree with referees that this violates the basic assumption of BIOME-BGC. A real month by month calibration as suggested by referee #1 (see the comment “R1C 2” below) is not possible in BIOME-BGC precisely because it is a dynamic vegetation simulator. Without modifying BIOME-BGC itself, we could only force BIOME-BGC to simulate more flexible state variables (such as leaf area index (LAI) and carboxylation capacity) in an artificial way (obtaining calibrated parameters for each month). The objective of this exercise was to identify the aspects of the model (i.e. relations between parameters and state variables) that may require improvement in order to better simulate the shape of the seasonal cycle of GPP. We acknowledge that this was not clear in the original manuscript, and we have elaborated this in the revision. Please see our response “**A1C 2**” below for more details.
2. The main idea behind the use of partitioned GPP instead of NEE data (measured on flux tower) directly in a Bayesian calibration was to tune the BIOME-BGC simulator parameters specifically for simulated GPP, which is the main output variable of interest in the paper. Please see our response “**A1C 3**” below for more details.

3. In the revised manuscript, we have deleted the section 4.4 and associated figures 5 and 6 of the previous manuscript following both referees' comments (**R1C 13** and **R2C 3** below). We have also added one extra figure (labelled Figure 3 in the revised manuscript) following referee's comment (**R1C 7** and **R2C 4** below)
4. We have deleted and revised some figures in the manuscript as follows:

Old figure number in the previous manuscript	New figure number in the revised manuscript	Remark
Figure 1	Figure 1	Both figures in the previous and revised manuscripts are same.
Figure 2	Figure 2	Both figures in the previous and revised manuscripts are same.
Figure 3	Figure 4	Figure 3 in the previous manuscript is revised following referee #1 comment <b>R1C 12</b> (see below)
Figure 4	Figure 5	Figure 4 in the previous manuscript is revised following referee #1 comment <b>R1C 12</b> (see below)
Figure 5	Removed	
Figure 6	Removed	
Figure 7	Figure 6	Figure 7 in the previous manuscript is revised following referee #1 comment <b>R1C 12</b> (see below)
Figure 8	Figure 7	Both figures in the previous and revised manuscripts are same.

5. We have extended table 3 (by adding one extra column for Experiment 1) to address referee #1 comment **R1C 1** (see below).

We look forward to hearing from you.

Yours sincerely

Dr Rahul Raj  
(On behalf of all authors)

## **Response to Referee #1 for “Bayesian integration of flux tower data into process-based simulator for quantifying uncertainty in simulated output” by R. Raj et al.**

We thank for the constructive and helpful comments for our manuscript. We have carefully considered all comments and these have incorporated in our revised manuscript accordingly. We have inserted our response to each comment. We use “R1C” for referee #1’s comment and “A1C” for author’s response to referee #1.

### Major concerns of Referee #1

#### **R1C 1:** On conclusion that temporal correlation matters

A control case without the correlation is missing. How do the results and implications change between accounting versus not accounting for correlations?

**A1C 1:** We ran the whole procedure without the temporal correlation in the residuals for Experiment 1. We found that both cases (accounting versus not accounting for correlations) led to similar temporal profile of the posterior simulated gross primary production (GPP) and similar values of statistical criteria (Root mean square error and Nash-Sutcliffe efficiency). The fact that the temporal correlation in the residuals is not only responsible for the temporal development of GPP indicated that the representation of dynamic processes within the BIOME-BGC simulator could be improved. We have added the new results of the control case without the correlation (see Figure 4 in the revised manuscript). We have explained the results in our revised manuscript (P7 L23-29, P8 L22, P12 L1-5, P13 L32-33, P14 L1-2, and P16 L3-8).

#### **R1C 2:** On conclusion about time varying parameters

I do not agree with the applied approach. In the presented study several independently simulated time series are mixed together. Each series includes the impact of changed parameters on the previous state. The parameter set valid for July was applied already to April, May, and June and affected the starting states of July. In my opinion one cannot conclude on time-varying parameters with this approach. The simulator needs to be run for the previous months also with the previous parameter set. The model state of the end of the month must be the starting state for the run of the next month with changed parameters. In an ideal case the entire time series would be run as one forward model and the combined (larger) parameter set would be estimated. A more feasible approach is to calibrate each month separately. For the next month calibration continues from a state of the previous month. This starting state needs to be drawn from the distribution of state vectors from the previous month posterior of states for each run with a new parameter sample. For the currently used method, at minimum, the forward runs that produce the predictive posterior and the fit statistics need to change the parameters across months in each single forward run to discuss seasonally changing parameters.

**A1C 2:** We are aware of the problems the reviewer identifies. We found that the response of simulated GPP to weather conditions is rather similar among months: The simulated GPP was mainly driven by the meteorology, and much less by seasonal phenology. We then hypothesized that some important state variables (such as LAI and carboxylation capacity) may not have a pronounced seasonal cycle in the model. Because these state variables are updated internally in the model, it is

not possible to perform a calibration per month: This would require changing the model code, and more importantly, it is in conflict with the main idea of the process simulator. In the second experiment we therefore calibrated the model to the data of each month separately, as if we had no information on GPP for the other months. If some of the parameters have different optimum values when calibrated to different months of data, then this is an indication that the relation between these parameters and important state variables that (should) change during the season, may require improvement.

By doing this experiment, we were able to identify the process that may require an improved description. We have mentioned above points in the revised manuscript (P14 L15-24, and P14 L25-35, and P15 L1-9). We decided to avoid the term 'time varying parameters' in the revision.

**R1C 3:** On using GPP to calibrate the mechanistic model

Net-ecosystem (NEE)-Flux-partitioned GPP is already the output of another statistical model – here the nonrectangular light response curve. This model already makes some strong process assumption e.g. on relationship of respiration with temperature. In effect the mechanistic model is calibrated against the output of another model. This makes it difficult to interpret the estimated parameters, their distribution and their meaning and process understanding. This needs to be discussed. Biome-BGC also computes respiration and NEE. You can compare these predictions to observations to gain additional insight into the model and the calibration. The flux partitioning also provides seasonally changing respiration at reference temperature and temperature sensitivity. Comparing these quantities to BIOME-BGC predictions lends further insight, which however, may also reveal sub-optimal calibration. A more direct way would be to include the respiration parts of the Biome-BGC model in the simulation and fit the simulated, i.e. predicted NEE to the NEE observations. Probably, this will introduce correlations in the joint posterior parameter estimates. But the weaker correlations in the presented GPP fit, are only resolved by the assumptions of the NEE-partitioning model that was used to derive GPP. While the presented GPP calibration has its own ground, those aspect needs to be addressed. The study would greatly benefit from a comparison to a calibration that uses NEE instead of GPP.

**A1C 3:** We would like to mention following points on using partitioned GPP instead of NEE data in this study:

- A. Indeed in our approach, the output of the process-based simulator was validated against the output of another model, notably the flux partitioning model. Although this approach has been used in other studies to validate the output of process-based simulator as well (Collalti et al., 2016, Liu et al., 2014, Yuan et al., 2014, Zhou et al., 2016), it could lead to error propagation. We clarify that the flux partitioning model (NRH model, Raj et al., (2016)) was tuned to the Eddy Covariance data in blocks of 10 days. Because the NHR and the relationship of respiration with temperature and moisture were tuned for these short blocks separately, we expect that the GPP still reflects realistic responses to environmental drivers, and does not depend much on model assumptions.
- B. Calibration of BIOME-BGC using NEE data is more challenging as NEE is the difference between fluxes caused by two processes (assimilation and respiration) We argue that calibration of such a complex model to NEE *instead* of GPP may not be a good idea, but calibration to NEE or respiration in addition to GPP is possible. However, we limited this study to the primary productivity, because this was our primary interest. A future study should be done to include both GPP data and ecosystem respiration data (can also be

achieved by partitioning of NEE data) in a Bayesian calibration of BIOME-BGC. This may ensure the accuracy of all related carbon budget terms (GPP, NEE, and respiration terms).

- C. As far as the comparison of simulated NEE and respiration with the measured NEE and partitioned respiration is concerned, this is out of the scope of the present study. We mainly focused on the simulated GPP and already presented a lot of results.

We have discussed all above points in our revised manuscript (P4 L18-22, and P15 L10-19).

**R1C 4:** On hitting the prior bound of residual uncertainty

Fig 1f clearly shows that the calibration tries to increase the residual variance and that high residual variances yields lower cost. In the current inversion, the residual variance is only bounded by the prior. This hints to deficiencies in the inversion. I sometimes experienced the same effect because a single equation of the cost (eq. 5) may in some cases not prefer the best fitting variance but the larger variance together with suboptimal parameters. Prescribing an upper bound is to my opinion not a good solution for this problem. Even fixing the residual variance would be a better option. My recommendation is to use several parameter blocks in a Metropolis within Gibbs sampling (Chib S Greenberg E (1995) Understanding the Metropolis-Hastings algorithm): One block to fit the model parameter conditional on the parameters of the residual statistical distribution and another block to fit the residual distribution parameters conditional on the current sample of model parameters.

**A1C 4:** We would like to clarify that SD in Fig 1 of the manuscript (both previous and revised manuscript) is not the residual variance. SD represents the effective soil depth and this is considered in this study as one of the parameters of BIOME-BGC simulator. In the figure caption, we have written that “Information about the BIOME-BGC parameters is given in Table 1”. We have specifically mentioned in the figure caption that “SD is effective soil depth” in the revised manuscript to avoid any confusion.

Further Concerns of Referee #1

**R1C 5:** The cut of the posterior by the edge of the prior distribution of LFRT and FRC:LC (Fig 1) shows inconsistency in the combination of the model, the prior knowledge, and the observations. This hints to deficiencies of the calibration. It also makes it difficult to interpret the parameter estimates and process understanding. This needs more discussion. The introduction of bias parameters in model drivers or model predictions could help to resolve the inconsistencies and, moreover, the bias parameters then can be interpreted.

**A1C 5:** Fig 1 shows the cut of the posterior by the edge of the prior distribution, which is called edge effect, of LFRT and FRC:LC. We agree that this clearly indicates a significant effect on our posterior parameter space of LFRT and FRC:LC by our particular choices of parameter space to be included in the prior distributions of LFRT and FRC:LC. It could be argued that the prior uniform distributions of LFRT and FRC:LC could be made wider in order to eliminate the edge effect. However, we did not do this for the following reasons:

- A. We carried out extensive literature review in a previous study (Raj et al., 2014) to compile the information on FRC:LC, LFRT, and other BIOME-BGC parameters. This information led to the characterization of uncertainty in the parameters and helped to define the prior distributions. For the present study, we used this information on prior distributions. We had no further scope to make the prior distributions wider at the study site.
- B. In the present study, we have used the upper limit of FRC:LC at 2.15. In our previous study (Raj et al., 2014) we found that higher values of FRC:LC led to disappearance of the forest (LAI=0) due to negative cumulative NEE, and hence no production at the study site. Therefore, we had no other choice of the upper limit of FRC:LC other than 2.16.

Further, we don't fully agree that the edge effect indicates deficiencies of the calibration. This can also be thought in another way that even if there is the edge effect, a drop in RMSE and enhancement in NSE coefficient (Table 3) before and after calibration indicated the efficiency of the calibration. We have mentioned above points in the revised manuscript (P10 L21-29, and P14 L5-7).

**R1C 6:** How were the initial states of the model prescribed?

**A1C 6:** Initial states of the model were prescribed with very low value ( $\approx 0$ ). Spin up simulation of BIOME-BGC was performed first to achieve steady state condition of soil carbon and nitrogen pools under given climate and site condition. Normal simulation was then started with these steady state condition using daily meteorological data of 2009. We have added these points in the revised manuscript (P4 L7-10).

**R1C 7:** Do you have correlations in the posterior parameter distribution, and how to you interpret them?

**A1C 7:** In the revised manuscript, we have added a brief explanation and a plot showing the correlations in the posterior parameter distribution obtained in Experiment 1 (Fig 3 and P10 L30-32, and P11 L1-8). We found a strong positive correlation between the posterior distributions of C:Nleaf (carbon and nitrogen ratio) and FLNR (Fraction of leaf N in Rubisco) with  $r=0.95$  ( $r$  is correlation coefficient). This strong positive correlation is in-line with the formulation of FLNR that shows direct proportionality with C:Nleaf (see Appendix A in RajEtal2014, for details). The parameters C:Nleaf and FLNR showed similar negative, but weak ( $> -0.5$ ), correlation with Wint (Canopy water interception coefficient) ( $r \approx -0.4$ ). This can be explained by the fact that the simulated GPP is expected to vary inversely with Wint via soil water potential and stomatal regulation and directly with FLNR and C:Nleaf (see Section 5.1 in the previous or revised manuscript, for details of BIOME-BGC internal routines). The parameter SD (effective soil depth) had similar positive, but weak ( $< 0.5$ ), correlation with FLNR and C:Nleaf ( $r \approx 0.4$ ). This can be explained by the fact that the simulated GPP is expected to vary directly with SD (via soil water potential and stomatal regulation), and FLNR and C:Nleaf. Two parameters of any other pair combinations did not show any notable correlation.

**R1C 8:** Please discuss your finding in the context of other studies that already performed a Bayesian calibration of BGC-models against Flux data. E.g. there is big body of studies using the DALEC model also looking at multiple constraints, model error, and different sources uncertainties.

**A1C 8:** We couldn't find papers on a Bayesian calibration of BIOME-BGC against flux data that compare with our results directly. We found other papers on calibration of BIOME-BGC, and one

study (Hidy et al., 2012) on Bayesian calibration of BIOME-BGC. Because Hidy et al. (2012) focussed on an herbaceous ecosystem, we could not compare directly the outcome quantitatively. .

#### Technical comments of Referee #1

**R1C 9:** Fig 1: Shows a very slow mixing. One chain needs more than 1000 steps to become uncorrelated with its previous state. Before computing the Gelman-Rubin criterion you should thin the chains by a factor so that autocorrelation or spectral density of the chain gets small.

**A1C 9:** We agree with the referee that thinning would reduce the spectral density of the chains. We decided not to do it again for the revised manuscript because we expect that thinning will not change the posterior estimations achieved in the study.

**R1C 10:** Fig 1: shortly explain phi and SD in the figure caption, e.g. “parameters describing variance and correlations of the distribution of model-data residuals (eq. 5)”

**A1C 10:** Please refer to our comment **A1C 4** on the clarification of SD. We have explained phi in the figure caption in the revised manuscript.

**R1C 11:** Fig 1: Maybe mention, that only the end of the chains after the burnin are shown.

**A1C 11:** Thank you very much for this suggestion. We have mentioned this in the figure caption in the revised manuscript.

**R1C 12:** Fig 3, . . . : Legends are missing. Please, use a different line type so that model and observations can be distinguished without color. Readers would benefit if you indicate months at the time axis instead of or in addition to Julian day.

**A1C 12:** We have modified the figure in the revised manuscript according to the referee’s suggestion.

**R1C 13:** Fig 6 and associated discussion: For a model with state variables or pools this result is trivial. I suggest omitting or explicitly elaborating on the magnitude of the impacts of state versus drivers on the model output and with witch conditions the one or the other becomes important.

**A1C 13:** We have omitted figure 6 in the revised manuscript.

**R1C 14:** P9L25ff: More discussion needed on hitting the upper prior boundaries and its consequences.

**A1C 14:** Please refer to our comment **A1C 5**.

**R1C 15:** P10L18: typo percentile

**A1C 15:** We have corrected this in the revised manuscript.

**R1C 16:** I cannot agree to the discussion because of the method that actually did not alter parameters across seasons during a single simulation run.

**A1C 16:** Please refer to our comment **A1C 2**.



## **Response to Referee #2 for “Bayesian integration of flux tower data into process-based simulator for quantifying uncertainty in simulated output” by R. Raj et al.**

We thank for the constructive and helpful comments for our manuscript. We have carefully considered all comments and these have incorporated in our revised manuscript accordingly. We have inserted our response to each comment. We use “R2C” for referee #2’s comment and “A2C” for author’s response to referee #2.

**R2C 1:** The main problem of this manuscript is the use of time-varying parameters. The authors themselves recognise this as a problem (see page 13, lines 11/12). If I understand their use of time-varying parameters correctly (‘engineering’ a times series of GPP based on independent monthly sub-time series) it actually violates Bayes theorem, mass conservation and model dynamics. Of course one can do such an experiment to better understand the model dynamics and identify missing or misrepresented processes, but the authors are not taking this step and analysing the consequences of their results with the time-varying parameters in terms of model structure and formulation.

**A2C 1:** We understand the concern of referee about the use time varying parameters. We found that the response of simulated GPP to weather conditions is rather similar among months: The simulated GPP was mainly driven by the meteorology, and much less by seasonal phenology. We then hypothesized that some important state variables (such as LAI and carboxylation capacity) may not have a pronounced seasonal cycle in the model. In the second experiment, we calibrated Biome-BGC to the GPP of each month separately, as if the data for the other months did not exist. In that way neither mass conservation nor the Bayes theorem is violated. If some of the parameters have different optimum values when calibrated to different months of data, then this is an indication that the relation between these parameters and important state variables that (should) change during the season, may require improvement. The problem only arises when we combine the results in a time series. We then merge different simulations outputs into one. The objective was indeed to better understand the dynamics (or lack of dynamics) of the model. We decided to avoid the term ‘time varying parameters’ in the revision. We have mentioned above points in the revised manuscript (P14 L15-24, and P14 L25-35, and P15 L1-9).

**R2C 2:** Another concern is the use of GPP derived from eddy-covariance flux measurements as the observations in the calibration process. Eddy-covariance towers measure the net exchange flux, essentially NEE, and GPP is the derived from this net flux by employing a model. So essentially, the authors calibrate the BIOME-BGC parameters against another model, in this case the NRH model which makes its own assumptions about the dependency of GPP on environmental conditions.

**A2C 2:** We would like to mention following points on using partitioned GPP instead of NEE data in this study:

- A. Indeed in our approach, the output of the process-based simulator was validated against the output of another model, notably the flux partitioning model. Although this approach has been used in other studies to validate the output of process-based simulator as well (Collalti et al., 2016, Liu et al., 2014, Yuan et al., 2014, Zhou et al., 2016), it could lead to error propagation. We clarify that the flux partitioning model (NRH model, Raj et al., (2016)) was tuned to the Eddy Covariance data in blocks of 10 days. Because the NHR and the

relationship of respiration with temperature and moisture were tuned for these short blocks separately, we expect that the GPP still reflects realistic responses to environmental drivers, and does not depend much on model assumptions.

- B. Calibration of BIOME-BGC using NEE data is more challenging as NEE is the difference between fluxes caused by two processes (assimilation and respiration) We argue that calibration of such a complex model to NEE *instead* of GPP may not be a good idea, but calibration to NEE or respiration in addition to GPP is possible. However, we limited this study to the primary productivity, because this was our primary interest. A future study should be done to include both GPP data and ecosystem respiration data (can also be achieved by partitioning of NEE data) in a Bayesian calibration of BIOME-BGC. This may ensure the accuracy of all related carbon budget terms (GPP, NEE, and respirations).

We have discussed all above points in the revised manuscript (P4 L18-22, and P15 L10-19).

**R2C 3:** The whole Section 4.4 is not needed and does not provide any new insights, it is obvious that a dynamical model with state variables such as BIOME-BGC then also depends on its state variables.

**A2C 3:** We have removed section 4.4 in the revised manuscript.

**R2C 4:** So essentially the remaining part of the manuscript concerns experiment 1 and becomes rather light-weighted as a thorough analysis of the results from experiment 1 is missing. For example, how does the posterior error covariance matrix look like and what consequences does this have on the parameters (identifiability) and model? How does the posterior uncertainty compare to prior uncertainty? What is the impact of the observations on other simulated quantities (NEE, NPP), both in terms of their mean and uncertainty? How does the variability and the temporal autocorrelation compare to the prior?

**A2C 4:**

- A. In the revised manuscript, we have added a brief explanation and a plot showing the correlations in the posterior parameter distribution obtained in Experiment 1 (Fig 3 and P10 L30-32, and P11 L1-8). We found a strong positive correlation between the posterior distributions of C:Nleaf (carbon and nitrogen ratio) and FLNR (Fraction of leaf N in Rubisco) with  $r=0.95$  ( $r$  is correlation coefficient). This strong positive correlation is in-line with the formulation of FLNR that shows direct proportionality with C:Nleaf (see Appendix A in RajEtal2014, for details). The parameters C:Nleaf and FLNR showed similar negative, but weak ( $> -0.5$ ), correlation with Wint (Canopy water interception coefficient) ( $r \approx -0.4$ ). This can be explained by the fact that the simulated GPP is expected to vary inversely with Wint via soil water potential and stomatal regulation and directly with FLNR and C:Nleaf (see Section 5.1 in the previous or revised manuscript, for details of BIOME-BGC internal routines). The parameter SD (effective soil depth) had similar positive, but weak ( $< 0.5$ ), correlation with FLNR and C:Nleaf ( $r \approx 0.4$ ). This can be explained by the fact that the simulated GPP is expected to vary directly with SD (via soil water potential and stomatal regulation), and FLNR and C:Nleaf. Two parameters of any other pair combinations did not show any notable correlation.

- B. We have already compared posterior and prior uncertainty in the section 4.2 of the previous manuscript (Fig 2 and P9 L22-25).
- C. As far as the impact of the observations on other simulated quantities (NEE, NPP) is concerned, this is out of the scope of the present study. We mainly focused on the simulated GPP and already presented a lot of results.
- D. This study modelled the temporal correlation in the residuals during the calibration by adding the nuisance parameter  $\phi$  in the likelihood function (see Section 3.3.2 in the previous manuscript). We had assumed uniform prior distribution of  $\phi$  between -1 and +1. In the posterior, we obtained the range of  $\phi$  from 0.56 to 0.93 with a mean at 0.75 (Fig 1g and P9 L15-18 in the previous manuscript). This showed the reduction in posterior uncertainty in  $\phi$  compared to prior. We have now mentioned the choice of prior uncertainty in  $\phi$  in the revised manuscript (P7 L19-20).

**R2C 5:** Also the terminology used in the manuscript is somewhat confusing. Sometimes the authors refer to simulated, sometimes to predicted GPP and sometimes to predicted flux tower GPP. In that context they also use the phrase ‘posterior flux tower GPP’, it is not clear to what the posterior refers?

A2C 5: We apologize for this confusion. We would like to clarify that the term “posterior” refers to the GPP obtained with posterior distribution of parameters. We agree that we had not used the terminology consistently. In the revised manuscript, we have made the terminology consistent as mentioned below:

- a. “Flux tower GPP” - We have now used this single term throughout the manuscript to indicate GPP partitioned from flux tower observation of net ecosystem exchange.
- b. “Posterior GPP” - We have now used this single term throughout the manuscript to indicate GPP simulated by BIOME-BGC at the posterior distribution of parameters.
- c. “Prior GPP” - We have now used this single term throughout the manuscript to indicate GPP simulated by BIOME-BGC at the prior distribution of parameters.
- d. “Simulated GPP” – Sometimes, we have used this term in the manuscript to give the general description of GPP simulated by BIOME-BGC irrespective of GPP simulated at prior or posterior distributions.

We have clarified this in the revised manuscript (P4 L17-18, P8 L12, P9 L26).

## References:

- Collalti, A., Marconi, S., Ibrom, A., Trotta, C., Anav, A., D'Andrea, E., Matteucci, G., Montagnani, L., Gielen, B., Mammarella, I., Grünwald, T., Knohl, A., Berninger, F., Zhao, Y., Valentini, R., and Santini, M.: Validation of 3D-CMCC forest ecosystem model (v.5.1) against eddy covariance data for 10 European forest sites, *Geoscientific Model Development*, 9, 479–504, 2016.
- Hidy, D., Barcza, Z., Haszpra, L., Churkina, G., Pintér, K., & Nagy, Z.: Development of the Biome-BGC model for simulation of managed herbaceous ecosystems, *Ecological Modelling*, 226, 99-119, 2012.
- Raj, R., Hamm, N. A. S., van der Tol, C., and Stein, A.: Variance-based sensitivity analysis of BIOME-BGC for gross and net primary production, *Ecological Modelling*, 292, 26–36, 2014.
- Raj, R., Hamm, N. A. S., van der Tol, C., and Stein, A.: Uncertainty analysis of gross primary production partitioned from net ecosystem exchange measurements, *Biogeosciences*, 13, 1409–1422, doi:10.5194/bg-13-1409-2016, 2016.
- Liu, D., Cai, W., Xia, J., Dong, W., Zhou, G., Chen, Y., Zhang, H., and Yuan, W.: Global validation of a process-based model on vegetation gross primary production using eddy covariance observations, *PLOS ONE*, 9, e110 407, 2014.
- Yuan, W., Cai, W., Xia, J., Chen, J., Liu, S., Dong, W., Merbold, L., Law, B., Arain, A., Beringer, J., Bernhofer, C., Black, A., Blanken, P. D., Cescatti, A., Chen, Y., Francois, L., Gianelle, D., Janssens, I. A., Jung, M., Kato, T., Kiely, G., Liu, D., Marcolla, B., Montagnani, L., Raschi, A., Rouspard, O., Varlagin, A., and Wohlfahrt, G.: Global comparison of light use efficiency models for simulating terrestrial vegetation gross primary production based on the LaThuile database, *Agricultural and Forest Meteorology*, 192–193, 108–120, 2014.
- Zhou, Y., Wu, X., Ju, W., Chen, J. M., Wang, S., Wang, H., Yuan, W., Andrew Black, T., Jassal, R., Ibrom, A., Han, S., Yan, J., Margolis, H., Rouspard, O., Li, Y., Zhao, F., Kiely, G., Starr, G., Pavelka, M., Montagnani, L., Wohlfahrt, G., D'Odorico, P., Cook, D., Arain, M. A., Bonal, D., Beringer, J., Blanken, P. D., Loubet, B., Leclerc, M. S. Y., Matteucci, G., Nagy, Z., Olejnik, J., Paw U, K. T., and Varlagin, A.: Global parameterization and validation of a two-leaf light use efficiency model for predicting gross primary production across FLUXNET sites, *Journal of Geophysical Research: Biogeosciences*, 121, 1045–1072, 2016.

# 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<sub>leaf</sub>), 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 **calibrating the BIOME-BGC to each month's flux tower GPP separately. As expected, the simulated GPP improved, but the calibrated parameter values also suggested that seasonal cycle of state variables could be improved.** ~~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<sub>2</sub> level. Knowledge of gross primary production (GPP) for forest ecosystems is indispensable for the estimation of forest carbon storage. Process-based 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 a 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~~ by calibrating the BIOME-BGC to the data of entire study period (growing season); and b) by calibrating the BIOME-BGC to 1 month of GPP data, and repeating the calibration for all months in the growing season.

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.

## 2 Site description

- 5 Calibration of BIOME-BGC was performed at the Speulderbos forest site, which is located at 52°15'08" N, 05°41'25" 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

### 10 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.

- 15 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
- 20 temperature, vapour pressure deficit, soil water content, solar radiation, atmospheric CO<sub>2</sub> 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. A 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
- 25 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
- 30 (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 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).

In this study, initial states of water, carbon, and nitrogen variables of the BIOME-BGC were prescribed with very low value ( $\approx 0$ ) as recommended in Thornton and Running (2002); Thornton et al. (2002). Spin up simulation of BIOME-BGC was performed first to achieve steady state condition of soil carbon and nitrogen pools under given climate and site condition. Normal simulation was then started with these steady state condition using daily meteorological data of 2009.

### 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 (hereafter, referred as flux tower GPP) and its associated uncertainty (2.5 percentiles, 97.5 percentiles, and medians). Posterior distribution of NRH parameters were obtained for every 10-day blocks in the growing season (Raj et al., 2016). Since the parameters may vary over time for example due to dependencies on the factors that are not included directly in the NRH model (e.g., soil moisture, canopy structure, and nutrient limitations). Hence, although these factors (that affect GPP) are not included in the model, they are accounted for implicitly by the calibration to 10-day blocks of data.

## 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 **flux tower** 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.

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

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

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

10 known with no uncertainty (Kennedy and O’Hagan, 2001).

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)

15 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  $\theta_j$ . Let the vector of simulator parameters  $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3, \dots, \theta_d)$ . 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  $\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \dots, \boldsymbol{\theta}^{(N)}$ . The following steps explain briefly the DREAM algorithms.

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

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

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

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  $i = 1, 2, 3, \dots, N$ :

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

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

and

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

where  $\delta$  is the number of chain pairs used to generate the candidate point,  $\theta^{(k)}$  and  $\theta^{(l)}$  are randomly selected from the state of other chains;  $k, l \in (1, 2, \dots, N)$  and  $k \neq l \neq i$ . The values of  $\lambda_d$  and  $\zeta_d$  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  $c = 10^{-6}$ .  $\gamma$  is the jump-size, whose value depends on  $\delta$  and  $d$ . DREAM implements a randomized subspace sampling, i.e., all dimensions of  $\theta^{(i)}$  are not updated jointly and some dimensions of  $\theta^{(i)*}$  are reset to those of  $\theta^{(i)}$ . The value of  $\gamma$  is, therefore, obtained with  $d'$ , the number of dimensions updated jointly.

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

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

(d) The candidate point  $\theta^{(i)*}$  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  $\theta^{(i)*}$  with a lower likelihood than the current candidate point.

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

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 are discarded as "burn-in" and the post burn-in samples are then used to conduct inference on each  $\theta_j$ . The post burn-in samples are then used to conduct inference on each  $\theta_j$ . For example median and 95 % credible interval can be obtained over these samples. A simulator is run on the posterior distributions of  $\theta$  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).

5

[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 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:

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

where  $\phi$  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  $\phi$  were different from zero (Section 4.1). **A uniform prior distribution of  $\phi$  between -1 and +1 was chosen as recommended in Vrugt (2016).**

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  $\mathbf{y}$ .

**If the error residuals are assumed to be uncorrelated, Eq. 5 reduces to the following equation:**

$$p_{\log}(\mathbf{z}|\boldsymbol{\theta}) = -\frac{n}{2}\log(2\pi) + -\sum_{t=1}^n \log(\hat{\sigma}_t) - \frac{1}{2} \sum_{t=1}^n \left( \frac{e_t}{\hat{\sigma}_t} \right)^2 \quad (6)$$

25

We also checked the changes in the results using the likelihood function not accounting for correlation in the residuals (Eq. 6). Mainly, the results, given below, were obtained using the likelihood function with temporal correlation in the residuals (Eq. 5). Whenever, we have presented the results using the likelihood function given by Eq. 6, we have specifically mentioned this.

### 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  $\theta_j$  ( $j = 1, 2, \dots, 6$  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  $\theta_j$ . 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  $\theta$ . BIOME-BGC was run at each parameter vector using daily meteorological data of 2009 and the daily simulated GPP (~~posterior prediction of GPP~~) (hereafter referred as **posterior GPP**) was evaluated and stored. This produced the distribution of daily posterior 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 posterior 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  $\theta$ :

1. Experiment 1: We used daily **mean of** 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 likelihood using Eq. (5), we set  $n = 153$ , equal to the 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  $\theta$  were used to ~~simulate~~ **obtain posterior** GPP and the associated uncertainty for each day in 2009. **The procedure of Experiment 1, stated above, were also repeated using the likelihood function given by Eq. 6.**
2. Experiment 2: We used daily **mean of** flux tower GPP for one month only, e.g., April, in the growing season to calibrate BIOME-BGC. For the calculation of likelihood **using Eq. (5)**, we set  $n = 30$ , equal to the number of days in April. The posterior samples of  $\theta$  were used to ~~simulate daily GPP with the associated uncertainty for 2009~~ **obtain posterior GPP and the associated uncertainty for each day in 2009**. We then extracted the daily ~~simulated~~ posterior GPP (with the associated uncertainty) of April only and discarded the other months in 2009. Likewise, we obtained ~~simulated~~ posterior 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  $\theta$ .

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  
5 GPP:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{t=1}^n (z_t - y_t)^2} \quad (7)$$

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

$$\text{NSE} = 1 - \frac{\sum_{t=1}^n (z_t - y_t)^2}{\sum_{t=1}^n (z_t - \bar{z})^2} \quad (8)$$

10 where  $\bar{z}$  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  $\text{NSE} \geq 0.5$  indicates adequate accuracy in the simulated GPP.

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

- 15 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  
20 flux tower GPP ( $z_{2.5}$  and  $z_{97.5}$ ).
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.
- 25 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 (hereafter referred as prior 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  $\theta_j$  obtained in both experiments (Table 2). Figures 1a to 1f show the trace plots of each  $\theta_j$  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  $\theta_j$  in each month of the growing season (trace plots not shown here). The visual and statistical diagnostic demonstrated that each  $\theta_j$  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  $\phi$ , 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  $\phi$  indicated that the residuals are temporarily correlated, thus supporting our choice of likelihood function (Eq. 5). For Experiment 2, non-zero values of  $\phi$  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  $\theta_j$  over the growing season for Experiment 2. **For Experiment 1, we obtained a single value for 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  $\theta_j$  was reduced compared to the prior distribution, indicating that  $\theta$  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, **which is called edge effect. Prior uniform distributions could be made wider in order to eliminate the edge effect. But,** 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 Dougl-fir at Speulderbos. **For FRC:LC, previous work (Raj et al., 2014) on the study area found the maximum limit of FRC:LC up to 6.85. But we did not use the limit of 6.85 to make the uniform distribution of FRC:LC wider in the present study. Raj et al. (2014) found that the increase of upper limit of the uniform distribution of FRC:LC from 2.16 to 6.85 led to the simulation with no development in LAI (leaf area index) and hence no production at the study site. The upper limit of FRC:LC at 2.16, however, fully supported the development of LAI at the study site. Therefore, we kept the upper limit of FRC:LC at 2.16 in the present study.**

A Bayesian calibration also allowed us to obtain correlation between the calibrated parameters. Figure 3 shows the correlation coefficients "r" and scatterplots between the posterior distributions of two parameters, obtained in Experiment 1, of different pair combinations. A strong positive correlation was found between the posterior distributions of C:N<sub>leaf</sub> and FLNR

with  $r = 0.95$ . This strong positive correlation is in-line with the formulation of FLNR that shows direct proportionality with  $C:N_{\text{leaf}}$  (see Appendix A in Raj et al., 2014, for details). The parameters  $C:N_{\text{leaf}}$  and FLNR showed similar negative, but weak ( $> -0.5$ ), correlation with  $W_{\text{int}}$  ( $r \approx -0.4$ ). This can be explained by the fact that the simulated GPP is expected to vary inversely with  $W_{\text{int}}$  via soil water potential and stomatal regulation and directly with FLNR and  $C:N_{\text{leaf}}$  (see Section 5.1, for details of BIOME-BGC internal routines). The parameter SD had similar positive, but weak ( $< 0.5$ ), correlation with FLNR and  $C:N_{\text{leaf}}$  ( $r \approx 0.4$ ). This can be explained by the fact that the simulated GPP is expected to vary directly with SD (via soil water potential and stomatal regulation), and FLNR and  $C:N_{\text{leaf}}$ . Two parameters of any other pair combinations did not show any notable correlation.

For Experiment 2, the uncertainties in LFRT, FRC:LC,  $W_{\text{int}}$ , 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 for calibration to GPP values of the peak of the growing season (July and 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  $W_{\text{int}}$ . The uncertainty in  $C:N_{\text{leaf}}$  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.]

[Figure 3 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. 4) and the validation period of September and October (Fig. 5). The daily simulated posterior GPP 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, daily posterior predicted daily GPP was close to flux tower GPP during the calibration period (Fig. 4), 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, posterior simulated GPP closely followed the flux tower GPP (Fig. 5).

The posterior predicted BIOME-BGC GPP was improved compared with the prior GPP predicted BIOME-BGC, as indicated by the drop of RMSE for the median as well as the 2.5 and 97.5 percentile 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 prior GPP after calibration.

We also evaluated the performance of calibrated BIOME-BGC using the likelihood function without the temporal correlation in the residuals (Eq. 6). The obtained daily medians of posterior GPP for the calibration period (April to August) are shown in Fig. 4. For daily medians as well as 2.5 and 97.5 percentile, RMSE and NSE criteria are shown in Table 3. We found that both likelihood functions Eq. 5 and Eq. 6 led to similar temporal profile of the posterior GPP and similar values of RMSE and NSE criteria.

[Figure 4 about here.]

[Figure 5 about here.]

[Table 3 about here.]

#### 4.4 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 6 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. 4). 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 6 about here.]

## 5 Discussion

### 5.1 Simulation 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. 7). These processes are implemented by different routines. The routines, however, are controlled not only by these six parameters, but also generate intermediate outputs, as shown in Fig. 7. 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 roots and stems (not shown in Fig. 7) together with leaves. The respiration terms are summed and then subtracted from GPP to obtain available carbon for allocation, which further updates leaf C. Finally, Fig. 7 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 7 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 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. 5), 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.~~ **It could be expected with  $\phi = 0$  that the simulator would properly capture the temporal development of GPP. However, this is not the case as shown in section 4.3. Both choices  $\phi \neq 0$  and  $\phi = 0$  led to**

similar posterior GPP. The fact that the residuals showed temporal correlation in the residuals is not only responsible for the temporal development of GPP 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 posterior GPP simulation as well as quantification of the associated uncertainty (Figs. 4 and 5). The edge effect in the posterior distributions of the parameters LFRT, FRC:LC, and SD (Section 4.2) could be seen as the deficiency of the calibration. A drop in RMSE and enhancement in NSE coefficient (Table 3) before and after calibration, however, indicated the efficiency of the calibration. Furthermore, the apparent overprediction of daily simulated posterior GPP, compared to flux tower GPP, for the month of April raised questions: (a) on the reliability of simulated posterior 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 for different months representing the phenological cycle 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 prediction of posterior GPP.

Consider Experiment 2. Note that BIOME-BGC actually simulated daily posterior GPP for a whole year with the posterior distributions of the parameters of each month. We selected only the daily simulated posterior GPP of that month to which the posterior distributions belong and we discarded other eleven months of simulations. The temporal profile in Fig. 6 is the combinations of daily simulated posterior GPP of each month in the growing season (Section 3.3.3 and 4.4). The resulting time series has discontinuities in state variables that can help to analyse the simulator behaviour in more detail. Thus the temporal profile of daily posterior GPP in Experiment 2 was obtained by mixing several independently simulated time series. Alternatively, one could think of updating the simulator state at the end of a month. This would then be the starting state for the run of the next month with changed parameters. This approach, however, is not possible in BIOME-BGC because it is a dynamic vegetation simulator. We could only force the BIOME-NGC to achieve more flexible state variables in an artificial way.

As expected, we observed an improvement (Fig. 6), particularly in the month of April, in the daily posterior predicted GPP compared to Experiment 1 (Fig. 4). 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. More interestingly, Experiment 2 showed variation in the six calibrated parameters depending on the month the BIOME-BGC was calibrated to (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 lowered lower  $W_{int}$  and higher SD, both increasing the soil water availability, in turn affecting the water intercepted by the canopy through the precipitation routing routine in Fig. 7. This suggests that either the soil water reservoir or the feedback mechanism between soil moisture and stomatal conductivity via the soil water potential was responsible for the underestimate of simulated GPP in Experiment 1. The parameters FRC:LC and LFRT also increased

and were also higher when calibrated to summer months. Both parameters both affect GPP through LAI. The variation in FLNR and  $C:N_{\text{leaf}}$ , which together determine  $V_{\text{cmax}}$ , also changed month-by-month (Fig. 7). These results indicate 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 LAI and  $V_{\text{cmax}}$ , at least in evergreen coniferous forest all state updates. These aspects may be studied in further detail by considering measurements of other state variables such as evaporation rates, soil moisture and LAI. The result was that the posterior predictive distribution of the parameters varied depending on the month used for calibration 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 limited the calibration to flux tower partitioned GPP. A limitation of this approach is that the output of process-based simulators is validated against the output of another model, notably the flux partitioning model. The latter is not a process model, but a semi-empirical model calibrated to 10-day's blocks of data. Although this approach has been used in many other studies that validate the output of process-based simulators (Collalti et al., 2016; Liu et al., 2014; Yuan et al., 2014; Zhou et al., 2016), it would also be possible to calibrate BIOME-BGC to other outputs such as evaporation rates and NEE. A calibration of BIOME-BGC using flux tower NEE data is more challenging as NEE is the difference between two fluxes (GPP and total respiration). Calibration to NEE alone does not guarantee that GPP and respiration terms are well calibrated (Mitchell et al., 2011). Here we decided to test the calibration algorithm for GPP first. The approach could however also be applied to additional state variables such as NEE or total respiration and water balance terms, in order to improve all carbon and water budget terms. Then, the number of parameters included in the calibration needs to be increased. In this study we performed our calibration based on six parameters (LFRT, FRC:LC,  $C:N_{\text{leaf}}$ ,  $W_{\text{int}}$ , 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 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, could make a more comprehensive calibration to multiple outputs feasible in the near 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 posterior (predictive) 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,  $\phi$ , 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~~ Our results indicated that BIOME-BGC did not properly simulate the temporal profile development of GPP **either we assumed the temporal correlation in the residuals (with  $\phi \neq 0$ ) or we ignored this (with  $\phi = 0$ )**. 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~~ **monthly variation** in 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 **monthly variation in the BIOME-BGC** ~~time-varying~~ parameters. ~~This reinforces our previous conclusion. The implications of temporal correlation and time-varying parameters~~ These aspects 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, 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.umd.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 script 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 script 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.

5 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.

10 (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)

15 (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.

20 (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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## References

- Bastin, L., Cornford, D., Jones, R., Heuvelink, G. B. M., Pebesma, E., Stasch, C., Nativi, S., Mazzetti, P., and Williams, M.: Managing uncertainty in integrated environmental modelling: The UncertWeb framework, *Environmental Modelling & Software*, 39, 116–134, doi:10.1016/j.envsoft.2012.02.008, 2013.
- 5 Braakhekke, M. C., Wutzler, T., Beer, C., Kattge, J., Schruppf, M., Ahrens, B., Schöning, I., Hoosbeek, M. R., Kruijt, B., Kabat, P., and Reichstein, M.: Modeling the vertical soil organic matter profile using Bayesian parameter estimation, *Biogeosciences*, 10, 399–420, 2013.
- Churkina, G. and Running, S. W.: Contrasting climatic controls on the estimated productivity of global terrestrial biomes, *Ecosystems*, 1, 206–215, 1998.
- Collalti, A., Marconi, S., Ibrom, A., Trotta, C., Anav, A., D'Andrea, E., Matteucci, G., Montagnani, L., Gielen, B., Mammarella, I., Grünwald, T., Knohl, A., Berninger, F., Zhao, Y., Valentini, R., and Santini, M.: Validation of 3D-CMCC forest ecosystem model (v.5.1) against eddy covariance data for 10 European forest sites, *Geoscientific Model Development*, 9, 479–504, 2016.
- 10 Constable, J. V. H. and Friend, A. L.: Suitability of process-based tree growth models for addressing tree response to climate change, *Environmental Pollution*, 110, 47–59, 2000.
- Dumont, B., Leemans, V., Mansouri, M., Bodson, B., Destain, J. P., and Destain, M. F.: Parameter identification of the STICS crop model, using an accelerated formal MCMC approach, *Environmental Modelling & Software*, 52, 121–135, 2014.
- 15 Farquhar, G. D., von Caemmerer, S., and Berry, J. A.: A biochemical model of photosynthetic CO<sub>2</sub> assimilation in leaves of C<sub>3</sub> species, *Planta*, 149, 78–90, 1980.
- Gelfand, A. E. and Smith, A. F. M.: Sampling-based approaches to calculating marginal densities, *Journal of the American Statistical Association*, 85, 398–409, 1990.
- 20 Gelman, A. and Rubin, D. B.: Inference from iterative simulation using multiple sequences, *Statistical Science*, 7, 457–511, 1992.
- Gelman, A., Carlin, J. B., Stern, H. S., Dunson, D. B., Vehtari, A., and Rubin, D. B.: *Bayesian Data Analysis*, CRC press, Boca Raton, 2013.
- Gilmanov, T. G., Verma, S. B., Sims, P. L., Meyers, T. P., Bradford, J. A., Burba, G. G., and Suyker, A. E.: Gross primary production and light response parameters of four Southern Plains ecosystems estimated using long-term CO<sub>2</sub>-flux tower measurements, *Global Biogeochemical Cycles*, 17, 1071, 2003.
- 25 Hamm, N. A. S., Finley, A. O., Schaap, M., and Stein, A.: A spatially varying coefficient model for mapping air quality at the European scale, *Atmospheric Environment*, 102, 393–405, doi:10.1016/j.atmosenv.2014.11.043, 2015a.
- Hamm, N. A. S., Soares Magalhães, R. J., and Clements, A. C. A.: Earth observation, spatial data quality and neglected tropical diseases, *PLoS Neglected Tropical Diseases*, 9, e0004164, doi:10.1371/journal.pntd.0004164, 2015b.
- Hartig, F., Dyke, J., Hickler, T., Higgins, S. I., O'Hara, R. B., Scheiter, S., and Huth, A.: Connecting dynamic vegetation models to data - an inverse perspective, *Journal of Biogeography*, 39, 2240–2252, 2012.
- 30 Hastings, W. K.: Monte Carlo sampling methods using Markov chains and their applications, *Biometrika*, 57, 97–109, 1970.
- He, H., Liu, M., Xiao, X., Ren, X., Zhang, L., Sun, X., Yang, Y., Li, Y., Zhao, L., Shi, P., Du, M., Ma, Y., Ma, M., Zhang, Y., and Yu, G.: Large-scale estimation and uncertainty analysis of gross primary production in Tibetan alpine grasslands, *Journal of Geophysical Research: Biogeosciences*, 119, 466–486, 2014.
- 35 Kennedy, M. C. and O'Hagan, A.: Bayesian calibration of computer models, *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63, 425–464, doi:10.1111/1467-9868.00294, 2001.

- Liu, D., Cai, W., Xia, J., Dong, W., Zhou, G., Chen, Y., Zhang, H., and Yuan, W.: Global validation of a process-based model on vegetation gross primary production using eddy covariance observations, *PLOS ONE*, 9, e110407, 2014.
- Mäkelä, A., Landsberg, J., Ek, A. R., Burk, T. E., Ter-Mikaelian, M., Ågren, G. I., Oliver, C. D., and Puttonen, P.: Process-based models for forest ecosystem management: current state of the art and challenges for practical implementation, *Tree Physiology*, 20, 289–298, 2000.
- 5 Maselli, F., Chiesi, M., Fibbi, L., and Moriondo, M.: Integration of remote sensing and ecosystem modelling techniques to estimate forest net carbon uptake, *International Journal of Remote Sensing*, 29, 2437–2443, 2008.
- McNaughton, K. and Jarvis, P.: Predicting effects of vegetation changes on transpiration and evaporation, *Water deficits and plant growth*, 7, 1–47, 1983.
- Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E.: Equation of state calculations by fast computing machines, *The Journal of Chemical Physics*, 21, 1087–1092, 1953.
- 10 Minunno, F., van Oijen, M., Cameron, D. R., and Pereira, J. S.: Selecting parameters for Bayesian calibration of a process-based model: A methodology based on canonical correlation analysis, *SIAM/ASA Journal on Uncertainty Quantification*, 1, 370–385, 2013.
- Mitchell, S., Beven, K., Freer, J., and Law, B.: Processes influencing model-data mismatch in drought-stressed, fire-disturbed eddy flux sites, *Journal of Geophysical Research: Biogeosciences*, 116, 2011.
- 15 Monteith, J. L. and Unsworth, M. H.: *Principles of Environmental Physics*, Edward Arnold, Sevenoaks, UK, 2nd edn., 1990.
- Monteith, J. L. and Unsworth, M. H.: *Principles of Environmental Physics*, Academic Press, Burlington, Massachusetts, 3rd edn., 2008.
- Nash, J. E. and Sutcliffe, J. V.: River flow forecasting through conceptual models part I— A discussion of principles, *Journal of hydrology*, 10, 282–290, 1970.
- Raj, R., Hamm, N. A. S., van der Tol, C., and Stein, A.: Variance-based sensitivity analysis of BIOME-BGC for gross and net primary
- 20 production, *Ecological Modelling*, 292, 26–36, 2014.
- Raj, R., Hamm, N. A. S., van der Tol, C., and Stein, A.: Uncertainty analysis of gross primary production partitioned from net ecosystem exchange measurements, *Biogeosciences*, 13, 1409–1422, doi:10.5194/bg-13-1409-2016, 2016.
- Reinds, G. J., van Oijen, M., Heuvelink, G. B. M., and Kros, H.: Bayesian calibration of the VSD soil acidification model using European forest monitoring data, *Geoderma*, 146, 475–488, 2008.
- 25 Running, S. W.: Testing Forest-BGC ecosystem process simulations across a climatic gradient in Oregon, *Ecological Applications*, 4, 238–247, 1994.
- Running, S. W. and Hunt, E. R.: Generalization of a forest ecosystem process model for other biomes, BIOME-BGC, and an application for global-scale models, in: *Scaling physiological processes: Leaf to globe*, edited by Ehleringer, J. R. and Field, C. B., pp. 141–158, Academic Press, Inc. New York, 1993.
- 30 Starrfelt, J. and Kaste, O.: Bayesian uncertainty assessment of a semi-distributed integrated catchment model of phosphorus transport, *Environmental Science: Processes & Impacts*, 16, 1578–1587, 2014.
- Steingrover, E. G. and Jans, W. W. P.: *Physiology of forest-grown Douglas fir trees: Effect of air pollution and drought*, Tech. Rep. 94/3, IBN DLO, Institute for Forestry and Nature Research, Wageningen, the Netherlands, 1994.
- Su, Z., Timmermans, W. J., van der Tol, C., Dost, R., Bianchi, R., Gomez, J. A., House, A., Hajnsek, I., Menenti, M., Magliulo, V., Esposito,
- 35 M., Haarbrink, R., Bosveld, F., Rothe, R., Baltink, H. K., Vekerdy, Z., Sobrino, J. A., Timmermans, J., van Laake, P., Salama, S., van der Kwast, H., Claassen, E., Stolk, A., Jia, L., Moors, E., Hartogensis, O., and Gillespie, A.: EAGLE 2006- Multi-purpose, multi-angle and multi-sensor in-situ and airborne campaigns over grassland and forest, *Hydrology and Earth System Sciences*, 13, 833–845, 2009.

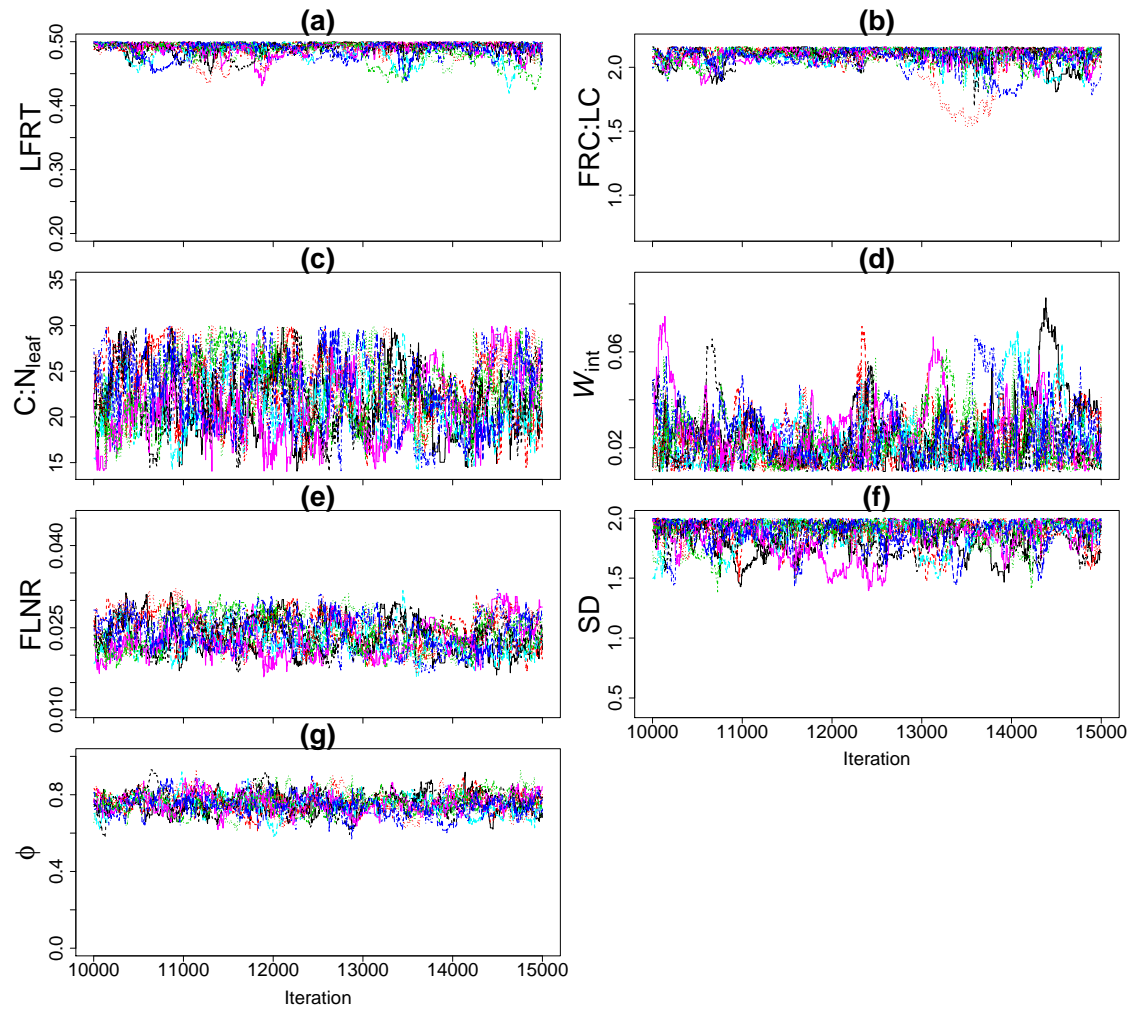
- Svensson, M., Jansson, P.-E., Gustafsson, D., Kleja, D. B., Langvall, O., and Lindroth, A.: Bayesian calibration of a model describing carbon, water and heat fluxes for a Swedish boreal forest stand, *Ecological Modelling*, 213, 331–344, 2008.
- Thornton, P.: Biome-BGC version 4.2: Theoretical Framework of Biome-BGC, Technical Documentation, 2010.
- Thornton, P. E.: Description of a numerical simulation model for predicting the dynamics of energy, water, carbon, and nitrogen in a terrestrial ecosystem, Ph.D. thesis, University of Montana, Missoula, 1998.
- 5 Thornton, P. E. and Running, S. W.: User's guide for Biome-BGC, Version 4.1.2, [http://www.ntsg.umt.edu/sites/ntsg.umt.edu/files/project/biome-bgc/bgc\\_users\\_guide\\_412.PDF](http://www.ntsg.umt.edu/sites/ntsg.umt.edu/files/project/biome-bgc/bgc_users_guide_412.PDF), 2002.
- Thornton, P. E., Law, B. E., Gholz, H. L., Clark, K. L., Falge, E., Ellsworth, D. S., Goldstein, A. H., Monson, R. K., Hollinger, D., Falk, M., Chen, J., and Sparks, J. P.: Modeling and measuring the effects of disturbance history and climate on carbon and water budgets in evergreen needleleaf forests, *Agricultural and Forest Meteorology*, 113, 185–222, 2002.
- 10 Ueyama, M., Ichii, K., Hirata, R., Takagi, K., Asanuma, J., Machimura, T., Nakai, Y., Ohta, T., Saigusa, N., Takahashi, Y., and Hirano, T.: Simulating carbon and water cycles of larch forests in East Asia by the BIOME-BGC model with AsiaFlux data, *Biogeosciences*, 7, 959–977, 2010.
- van Oijen, M., Rougier, J., and Smith, R.: Bayesian calibration of process-based forest models: bridging the gap between models and data, *Tree Physiology*, 25, 915–927, 2005.
- 15 van Oijen, M., Cameron, D. R., Butterbach-Bahl, K., Farahbakhshazad, N., Jansson, P. E., Kiese, R., Rahn, K. H., Werner, C., and Yeluripati, J. B.: A Bayesian framework for model calibration, comparison and analysis: Application to four models for the biogeochemistry of a Norway spruce forest, *Agricultural and Forest Meteorology*, 151, 1609–1621, 2011.
- van Oijen, M., Reyer, C., Bohn, F. J., Cameron, D. R., Deckmyn, G., Flechsig, M., Härkönen, S., Hartig, F., Huth, A., Kiviste, A., Lasch, P., Mäkelä, A., Mette, T., Minunno, F., and Rammer, W.: Bayesian calibration, comparison and averaging of six forest models, using data from Scots pine stands across Europe, *Forest Ecology and Management*, 289, 255–268, 2013.
- 20 van Wijk, M. T., Dekker, S. C., Bouten, W., Kohsiek, W., and Mohren, G. M. J.: Simulation of carbon and water budgets of a Douglas-fir forest, *Forest Ecology and Management*, 145, 229–241, 2001.
- Vrugt, J. A.: Markov chain Monte Carlo simulation using the DREAM software package: Theory, concepts, and MATLAB implementation, *Environmental Modelling & Software*, 75, 273–316, 2016.
- 25 Vrugt, J. A., ter Braak, C. J. F., Clark, M. P., Hyman, J. M., and Robinson, B. A.: Treatment of input uncertainty in hydrologic modeling: Doing hydrology backward with Markov chain Monte Carlo simulation, *Water Resources Research*, 44, 2008.
- Vrugt, J. A., ter Braak, C. J. F., Diks, C. G. H., Robinson, B. A., Hyman, J. M., and Higdon, D.: Accelerating Markov chain Monte Carlo simulation by differential evolution with self-adaptive randomized subspace sampling, *International Journal of Nonlinear Sciences and Numerical Simulation*, 10, 273–290, 2009.
- 30 White, M., Thornton, P., Running, S., and Nemani, R.: Parameterization and sensitivity analysis of the BIOME-BGC terrestrial ecosystem model: Net primary production controls, *Earth Interactions*, 4, 1–85, 2000.
- Xenakis, G., Ray, D., and Mencuccini, M.: Sensitivity and uncertainty analysis from a coupled 3-PG and soil organic matter decomposition model, *Ecological Modelling*, 219, 1–16, 2008.
- 35 Yan, M., Li, Z., Tian, X., Chen, E., Zhang, W., Guo, Y., and Li, C.: Simulation of carbon flux of forest ecosystem by BIOME-BGC and MODIS-PSN models, in: 2014 IEEE Geoscience and Remote Sensing Symposium, pp. 1065–1068, 2014.
- Yuan, W., Cai, W., Xia, J., Chen, J., Liu, S., Dong, W., Merbold, L., Law, B., Arain, A., Beringer, J., Bernhofer, C., Black, A., Blanken, P. D., Cescatti, A., Chen, Y., Francois, L., Gianelle, D., Janssens, I. A., Jung, M., Kato, T., Kiely, G., Liu, D., Marcolla, B., Montagnani,



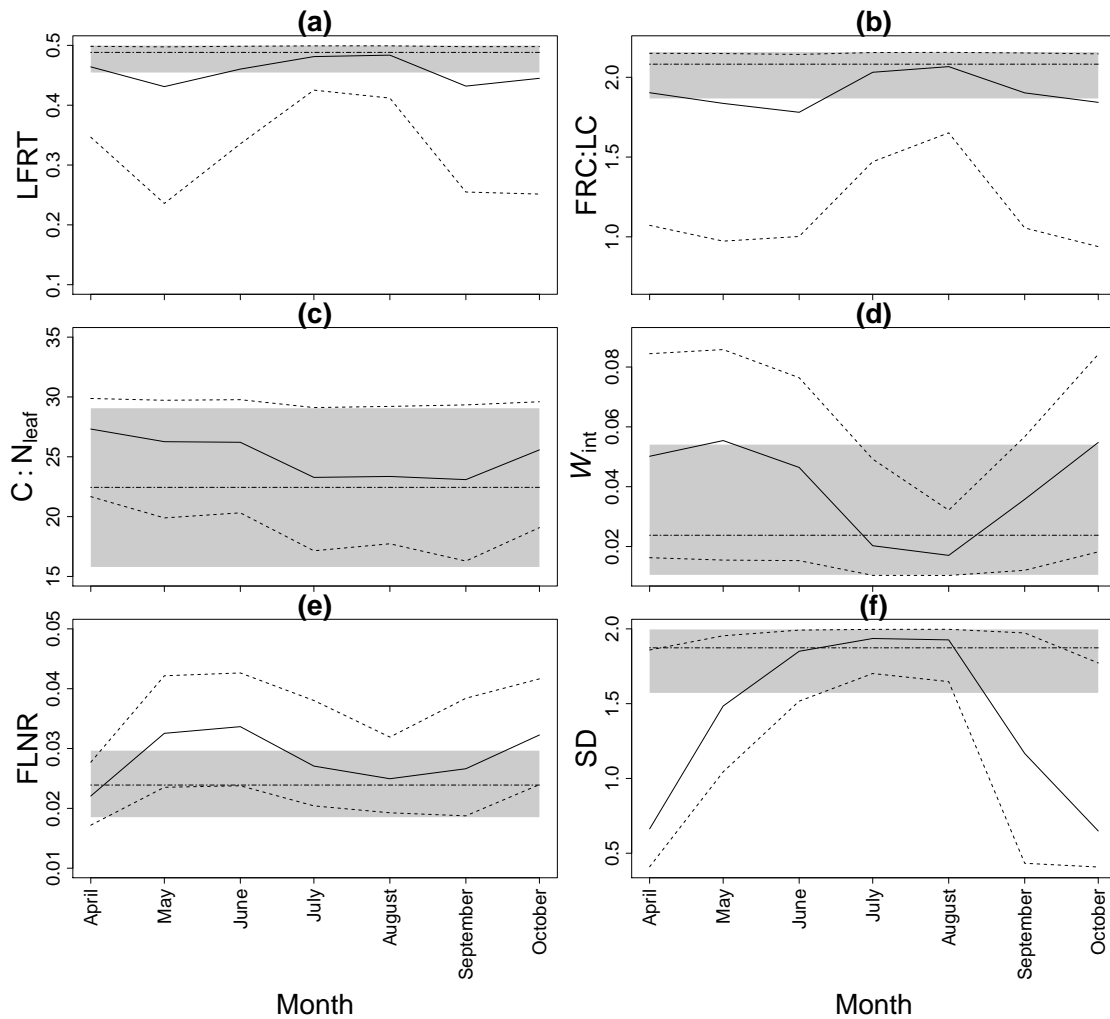
- L., Raschi, A., Roupsard, O., Varlagin, A., and Wohlfahrt, G.: Global comparison of light use efficiency models for simulating terrestrial vegetation gross primary production based on the LaThuile database, *Agricultural and Forest Meteorology*, 192—193, 108–120, 2014.
- 5 Zhou, Y., Wu, X., Ju, W., Chen, J. M., Wang, S., Wang, H., Yuan, W., Andrew Black, T., Jassal, R., Ibrom, A., Han, S., Yan, J., Margolis, H., Roupsard, O., Li, Y., Zhao, F., Kiely, G., Starr, G., Pavelka, M., Montagnani, L., Wohlfahrt, G., D’Odorico, P., Cook, D., Arain, M. A., Bonal, D., Beringer, J., Blanken, P. D., Loubet, B., Leclerc, M. Y., Matteucci, G., Nagy, Z., Olejnik, J., Paw U, K. T., and Varlagin, A.: Global parameterization and validation of a two-leaf light use efficiency model for predicting gross primary production across FLUXNET sites, *Journal of Geophysical Research: Biogeosciences*, 121, 1045–1072, 2016.

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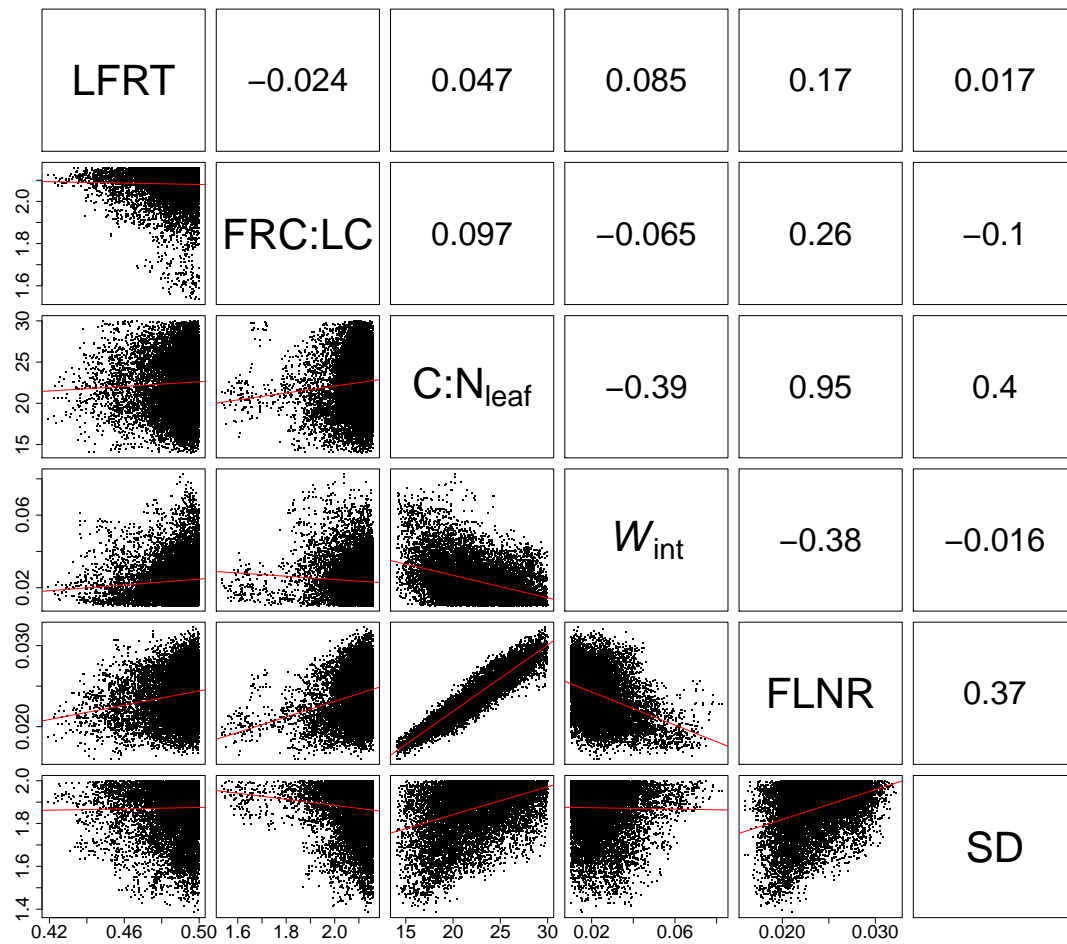
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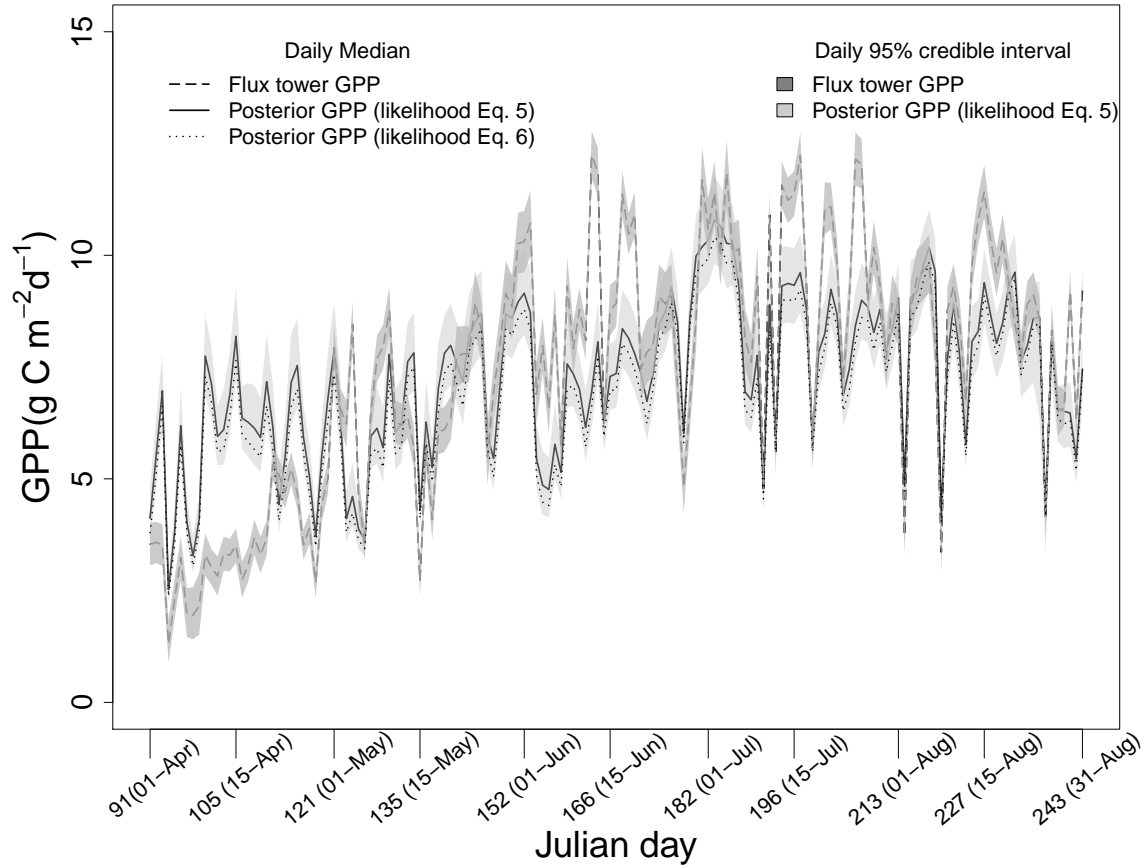
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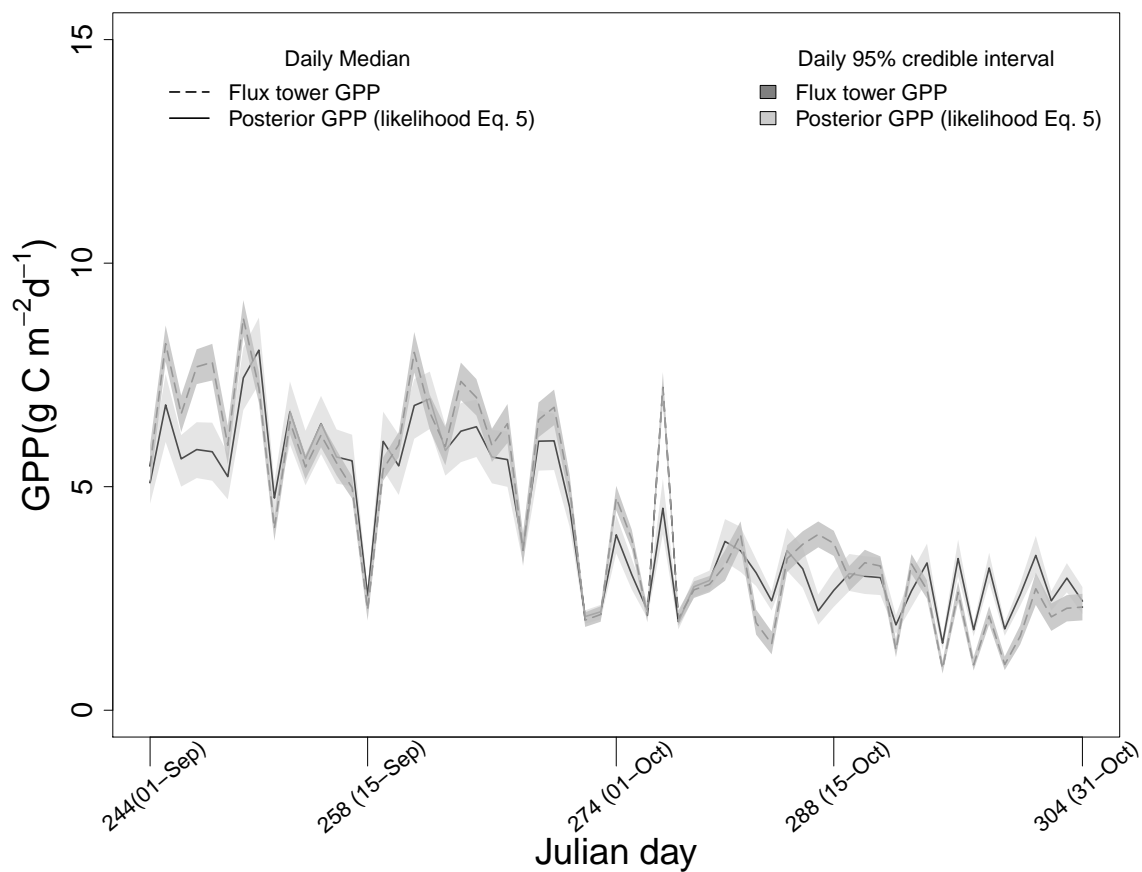
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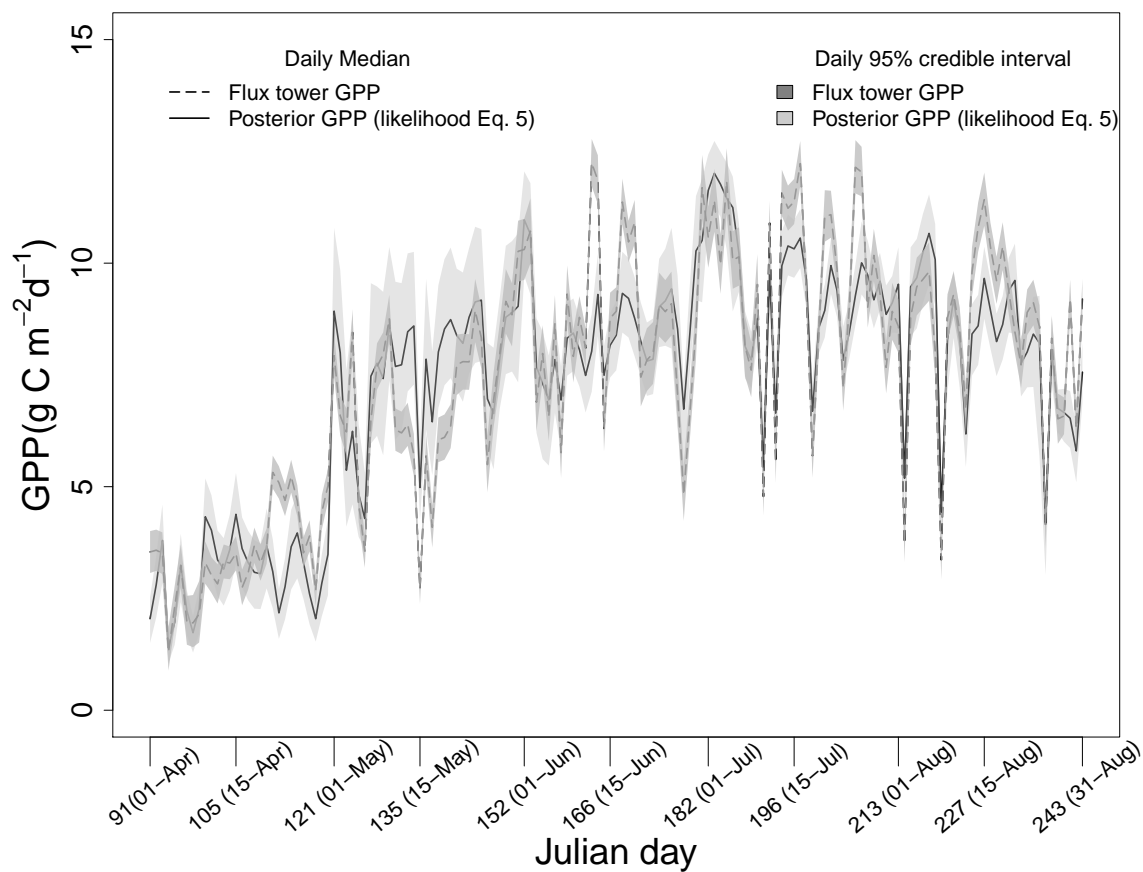
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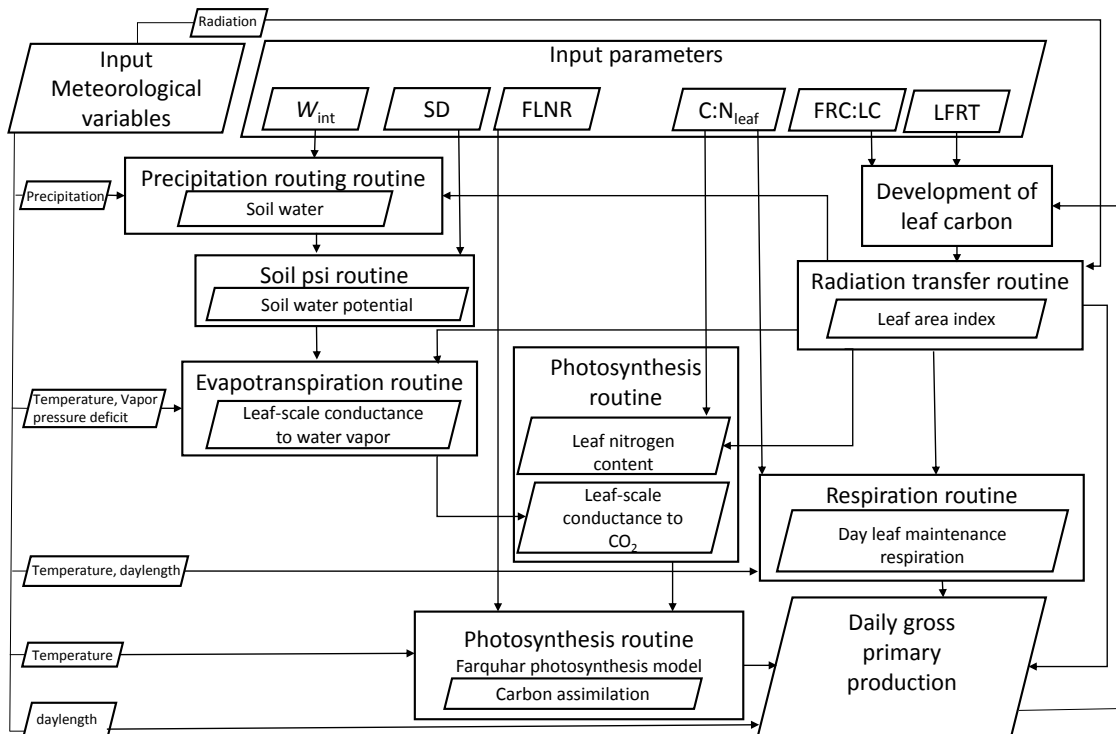


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Ecophysiological parameter	Symbol	Unit	Mean value/distribution <sup>†</sup>
<b>Leaf and fine root turnover</b>	<b>LFRT</b>	$1 \text{ yr}^{-1}$	$U(0.196, 0.5)^{\dagger}$
Annual live wood turnover fraction	LWT	$1 \text{ yr}^{-1}$	0.70
Annual whole-plant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

**Table 2.** Gelman–Rubin potential scale reduction factor (PSRF) of each BIOME-BGC parameter selected for calibration and  $\phi$  (nuisance parameter of likelihood function Eq. 5) for experiment 1 and 2. Information about the BIOME-BGC parameters is given in Table 1. SD is effective soil depth

		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 <sub>leaf</sub>		1.04	1.02	1.02	1.01	1.04	1.04	1.03	1.03
W <sub>int</sub>		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
$\phi$		1.02	1.03	1.01	1.01	1.03	1.03	1.01	1.01

**Table 3.** Root mean square error (RMSE) and Nash-Sutcliffe efficiency (NSE) between the **prior (before calibration)/posterior** predicted BIOME-BGC GPP and flux tower GPP for different experiments (see Section 3.3.4) and **likelihoods (see Section 3.3.2)**.

	Period	2.5%		Median		97.5%	
		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 (With likelihood Eq. 5)	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 1 (With likelihood Eq. 6)	April to August	1.82	0.54	1.87	0.54	1.94	0.52
Experiment 2 (With likelihood Eq. 5)	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