

Improving the predictability of global CO₂ assimilation rates under climate change

T. Ziehn,¹ J. Kattge,² W. Knorr,^{1,3} and M. Scholze¹

Received 24 February 2011; revised 14 April 2011; accepted 14 April 2011; published 27 May 2011.

[1] Feedbacks between the terrestrial carbon cycle and the atmosphere have the potential to greatly modify expected rates of future climate change. This makes it all the more urgent to exploit all existing data for the purpose of accurate modelling of the underlying processes. Here we use a Bayesian random sampling method to constrain parameters of the Farquhar model of leaf photosynthesis and a model of leaf respiration against a comprehensive set of plant trait data at the leaf level. The resulting probability density function (PDF) of model parameters is contrasted with a PDF derived using a conventional “expert knowledge” approach. When running the Biosphere Energy Transfer Hydrology (BETHY) scheme with a 1000-member sub-sample of each of the two PDFs for present climate and a climate scenario, we find that the use of plant trait data is able to reduce the uncertainty range of simulated net leaf assimilation (NLA) by more than a factor of two. Most of the remaining variability is caused by only four parameters, associated with the acclimation of photosynthesis to plant growth temperature and to how leaf stomata react to atmospheric CO₂ concentration. We suggest that this method should be used extensively to parameterize Earth system models, given that data bases on plant traits are increasingly being made available to the modelling community. **Citation:** Ziehn, T., J. Kattge, W. Knorr, and M. Scholze (2011), Improving the predictability of global CO₂ assimilation rates under climate change, *Geophys. Res. Lett.*, 38, L10404, doi:10.1029/2011GL047182.

1. Introduction

[2] The terrestrial carbon balance has a great impact on present and future levels of atmospheric carbon dioxide (CO₂). The effect by which warming causes levels of CO₂ to rise which in turn causes further warming has been described as a climate-carbon cycle feedback. Predictions of the terrestrial carbon balance still vary significantly due to differences between models [Cramer *et al.*, 1999; Friedlingstein *et al.*, 2006], and due to uncertainties of the process parameters of the terrestrial ecosystem models (TEMs) [Knorr and Heimann, 2001], with parameters related to photosynthesis and leaf respiration being among the most sensitive ones [Zaehle *et al.*, 2005]. First attempts have been conducted to constrain the parameters of TEMs by inversion

against eddy covariance measurements of CO₂ and energy fluxes [Wang *et al.*, 2001; Braswell *et al.*, 2005; Knorr and Kattge, 2005; Santaren *et al.*, 2007] and on a global scale by inversion against atmospheric CO₂ concentration measurements [Rayner *et al.*, 2005]. In this context, the Bayesian approach has been proven to be a convenient and powerful method as it combines prior knowledge about parameters with additional information gained from the inversion in a consistent and accountable way [Rayner *et al.*, 2005]. Nonetheless, parameter estimates in Earth system models used to simulate the strength of the climate-carbon cycle feedback are still mostly based on rather subjective “expert knowledge”. For that reason, we here apply a more objective method of parameter constraint based on model inversion against a large amount of observations, both for model parameter values and values assigned to model output.

[3] In this contribution, model inversion is based on a Markov Chain Monte Carlo (MCMC) method, where the probability density function (PDF) of parameters is sampled directly [Knorr and Kattge, 2005]. We simulate net leaf assimilation (NLA), defined as gross photosynthesis minus leaf-level respiration, at the global scale and how it varies with model parameters across time. NLA is a major part of the global terrestrial carbon balance and more reliable projections of NLA are urgently needed to better quantify the strength of the climate-carbon cycle feedback.

2. Material and Methods

[4] We use an extended version of Farquhar *et al.*'s [1980] photosynthesis model and a Bayesian approach to combine different kinds of data at the leaf level to derive a consistent parameterization of 41 parameters. All parameters of the model, apart from photosynthetic capacity, which is dependent on plant functional type (PFT), are assumed to be general for higher plants with C3-type photosynthesis [von Caemmerer, 2000] and have one value globally. Even though they show considerable variability between species [Yeoh *et al.*, 1981], their use as global parameters in models is firmly established, while their variability has never been evaluated in a systematic fashion.

2.1. Photosynthesis Model

[5] For C3 photosynthesis we use a substantial extension of Farquhar *et al.*'s [1980] model following Medlyn *et al.* [1999], with a parametrization of Rubisco kinetics and temperature dependence of photosynthesis according to Bernacchi *et al.* [2001]. Acclimation of photosynthesis and respiration to plant growth temperature is taken into account following Kattge and Knorr [2007], while C4 photosynthesis is calculated according to Collatz *et al.* [1992]. Photosynthetic capacity is related to leaf nitrogen content [Medlyn

¹Department of Earth Sciences, University of Bristol, Bristol, UK.

²Max-Planck Institute for Biogeochemistry, Jena, Germany.

³Department of Meteorology and Climatology, Aristotle University of Thessaloniki, Thessaloniki, Greece.

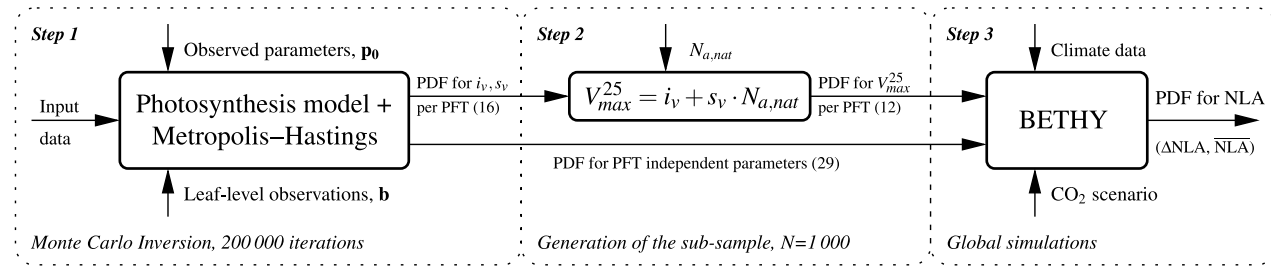


Figure 1. Flow chart of the assimilation scheme and the simulation of the sub-sample with BETHY based on the derived posterior parameter PDF. The number of estimated parameters is given in parentheses.

et al., 1999; Kattge *et al.*, 2009]. Temperature dependence of leaf respiration is modelled by a Q_{10} approach according to Tjoelker *et al.* [2001], which has been modified here for the use in process models accounting for the observed decline of temperature sensitivity with increasing leaf temperature. Q_{10} is the relative increase in the respiration rate for 10°C of temperature rise. All model equations are provided in detail in the auxiliary material.¹

[6] With respect to compatibility to global terrestrial ecosystem models, we use this conservative formulation of photosynthesis and respiration and do not accounting for phosphorous deficiency, leaf ageing, different temperature sensitivities of respiration in light and in the dark and mesophyll conductance.

2.2. Parametrization Scheme

[7] We distinguish between prior and posterior PDFs. The prior PDF is defined by an expert knowledge approach using published parameter values to estimate mean and standard error of parameter values (see Tables S3 and S4). The posterior PDF combines more extensive prior knowledge about parameter values, derived from a trait data base, with how well simulations with those parameters match observed leaf-level observations (photosynthesis, respiration and stomatal conductance, see Table S2).

[8] In the Bayesian context used in this study, the posterior PDF of parameters, $f(\mathbf{p})$, is expressed as the product of the PDF derived from observed parameter values, $\rho_0(\mathbf{p})$, the likelihood function $L(\mathbf{p})$ which measures the deviation between measured and simulated leaf-level observations, and a normalization constant, ν :

$$f(\mathbf{p}) = \nu \rho_0(\mathbf{p}) L(\mathbf{p}). \quad (1)$$

$\rho_0(\mathbf{p})$ describes the mismatch between the optimized parameters and the observed parameters. The likelihood function $L(\mathbf{p})$ characterises the misfit of modelled values against leaf-level observations (see Table S2). Uncertainties in the observed parameters and the leaf-level observations are included via their error covariance matrix. All uncertainties are assumed to be Gaussian. Covariances between observations and errors due to missing or incorrect processes in the model are not considered.

[9] To compute appropriate samples of model parameter values that approximate the PDF of posterior parameter

values, $f(\mathbf{p})$, we use the Metropolis-Hastings algorithm (MCMC method), which is based on an acceptance-rejection strategy. The parameter estimates and uncertainties are derived as follows: All parameters are constrained simultaneously against observations of model parameter values (via ρ_0) and observations of leaf-level photosynthesis rates (via L , more details regarding the observations are provided in the auxiliary material). We thus obtain the PDF for 29 model parameters independent of PFT and 16 PFT dependent parameters (slope s_V and intercept i_V for the nitrogen use efficiency). The constrained linear relationship of V_{\max}^{25} (maximum carboxylation rate at 25°C) to leaf nitrogen content, $N_{a,nat}$, which we obtain from the Monte Carlo inversion is then used to infer V_{\max}^{25} for 12 PFTs (see Figure 1, step 2). This enables us to use a much larger dataset of leaf nitrogen content in natural environment, $N_{a,nats}$ for the estimation of V_{\max}^{25} . This approach has been described in detail by Kattge *et al.* [2009].

[10] While the uncertainties of observations are represented within the likelihood function and the probability distribution of parameters, the uncertainties of model input data (see auxiliary material) are taken into account during Monte Carlo sampling [Kattge *et al.*, 2009]. In this method, the distribution of each model input value is assumed to be Gaussian. Within each iteration of the MCMC sequence, one representation of this distribution is selected according to its intrinsic probability. The high number of MCMC iterations (200000) thus produces an adequate representation of the probability density distribution of each input value and thus of $f(\mathbf{p})$ reflecting input data uncertainty.

2.3. Model Setup

[11] The Biosphere Energy Transfer Hydrology (BETHY) scheme is used to simulate leaf-level carbon fluxes for a sub-sample of the PDF of the prior (expert knowledge) and the posterior parameter values (step 3 in Figure 1). BETHY is run on a $2^\circ \times 2^\circ$ grid with 3462 land grid cells (excl. Antarctica). Global vegetation is mapped onto 12 different PFTs (see Table S4) and each grid cell can contain up to three sub-grid cells with different PFTs. In this study, BETHY is driven by present climate data and a climate scenario from the Hadley Centre Coupled Model, version 3 (HadCM3) over 121 years for the period 1979 to 2099. Atmospheric CO₂ concentrations are based on the A2 scenario of Intergovernmental Panel on Climate Change [2001] over the simulation period. A more detailed description of BETHY is given by Knorr and Heimann [2001].

¹Auxiliary materials are available in the HTML. doi:10.1029/2011GL047182.

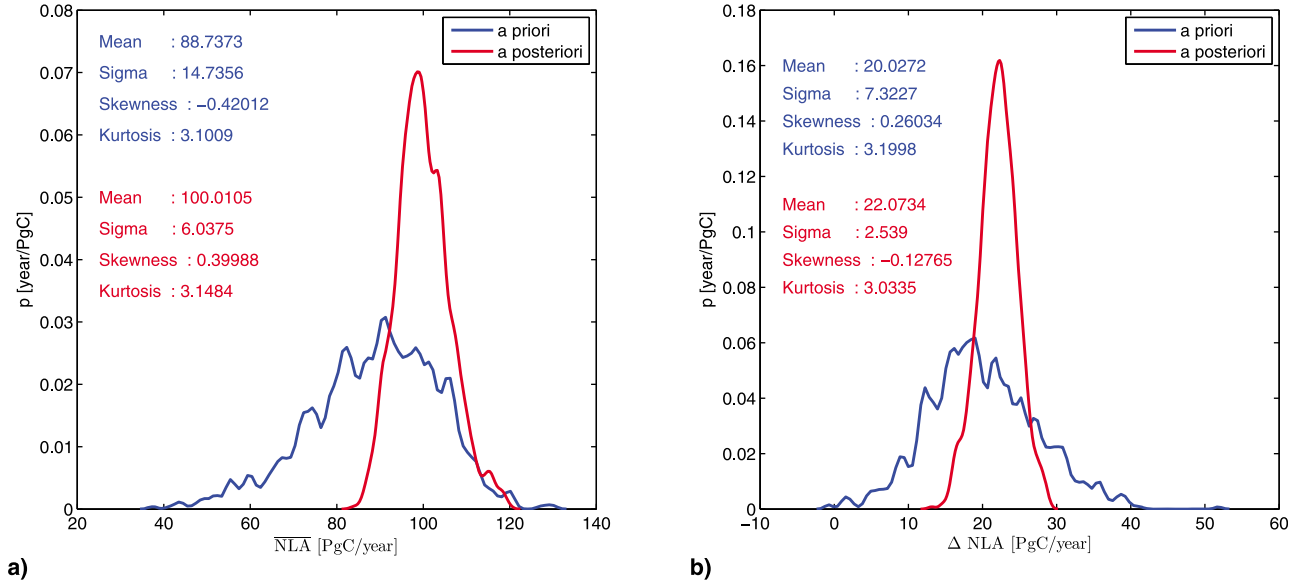


Figure 2. Probability density function estimate of (a) mean NLA over the first 20 simulation years (\overline{NLA}) and (b) ΔNLA (difference of mean NLA last 20 years and mean NLA first 20 years) based on 1000 randomly sampled prior parameter values (expert knowledge) and 1000 posterior parameter values drawn from the MCMC sequence. The estimate is based on a normal kernel function, using a bandwidth of 1 (Figure 2a) and 0.5 (Figure 2b) respectively.

[12] A sub-sample size of $N = 1000$ is used in both prior and posterior cases. For the prior parameter sub-sample we draw random values for all parameters, from a Gaussian distribution with a mean and standard error as provided in Tables S3 and S4.

[13] In order to generate the sub-sample for the posterior parameters we use every 150th sample from the MCMC sequence for the parameters independent of PFT leaving out the first 50000 iterations. Each realisation of the PFT dependent parameter V_{\max}^{25} is calculated using a representation of $N_{a,nat}$ and every 150th parameter set of the intercept i_V and slope s_V as sampled by the MCMC algorithm (step 2 in Figure 1):

$$V_{\max}^{25} = i_V + s_V \cdot N_{a,nat} \quad (2)$$

We consider the uncertainty in $N_{a,nat}$ by randomly selecting values from a Gaussian distribution with the standard error and mean of $N_{a,nat}$ as presented in Table S4. Due to the fact that we do not have any data available for $N_{a,nat}$ for one PFT (tundra vegetation), we use random values with the same mean and standard deviation as in the prior case. Therefore, we are not able to gain any information for the posterior value of V_{\max}^{25} for this PFT.

3. Results and Discussion

[14] In order to compare our results with independent data, we calculate the gross primary productivity (GPP) on a global scale from the BETHY ensemble runs for both cases. According to Beer *et al.* [2010], the observation based estimate of this flux is 123 PgC/yr for the period 1998 to 2005 with a 95% confidence interval from 102 to 135 PgC/yr. The range reflects differences in the way eddy covariance data are extrapolated to the global land surfaces. With the prior parameter sub-sample we calculate a smaller global

GPP of 107.42 PgC/yr for the same period with a 95% confidence interval from 65.52 to 126.69 PgC/yr. The lower range of the confidence interval is much smaller than the one from the observation based estimate, which shows that we tend to underestimate GPP with the unconstrained photosynthesis model in BETHY. In contrast to this, the ensemble runs based on the posterior parameter values produce a better match with the observation based estimates. Global GPP is now 121.04 PgC/yr with a 95% confidence interval from 110.07 to 129.94 PgC/yr which is in good agreement with the global estimate based on eddy covariance flux data from Beer *et al.* [2010].

[15] In this study, we focus on two characteristics of net leaf assimilation (NLA): The first one is mean NLA per year over the first 20 years of the simulation period (\overline{NLA}), the second is the difference between mean NLA over the last 20 and mean NLA over the first 20 simulation years (ΔNLA).

[16] Figure 2a shows the PDF of \overline{NLA} for both cases. Both distributions can be approximated very well by a Gaussian as indicated by skewness and kurtosis (note: kurtosis of the normal distribution is 3). The mean value in the posterior case is slightly larger than in the prior case. However, the uncertainty is reduced by more than a factor of two, from $\sigma = 14.74$ to $\sigma = 6.04$ if using the posterior parameter values. We find similar results when analysing the PDF of ΔNLA (Figure 2b). Again, the distribution in both cases is approximately Gaussian and the mean values are nearly the same. The uncertainty, however, is reduced by nearly a factor of three, from $\sigma = 7.32$ to $\sigma = 2.54$, between using the prior and the posterior parameter values. This demonstrates clearly the usefulness of our approach to apply plant trait data to constrain parameters of the photosynthesis model.

[17] A sensitivity analysis performed via a simple statistical correlation analysis between each sample's parameter value and the resulting value for the target quantity ΔNLA

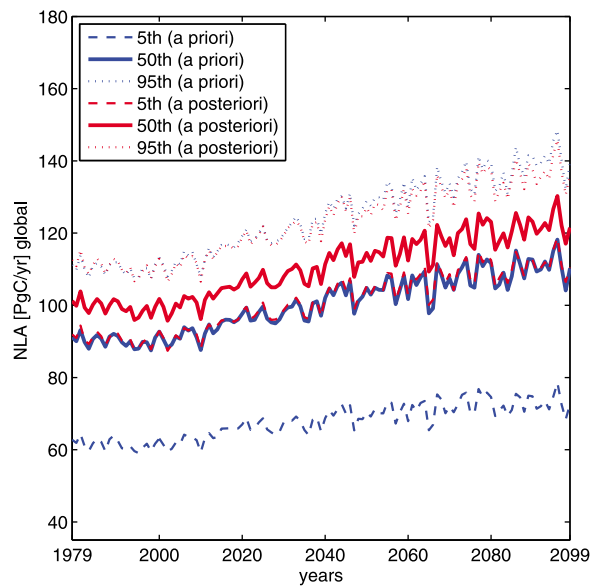


Figure 3. Percentiles of NLA for each year based on 1000 randomly sampled prior parameter values (expert knowledge) and 1000 posterior parameter values drawn from the MCMC sequence.

can be used to identify the main contributing parameters responsible for the uncertainty of the target quantity. Taking R^2 (the square of the Pearson correlation coefficient) as the coefficient of determination, the following four dominant parameters were identified: $s\Delta S_{Jm}$ ($R^2 = 0.40$), $sf_{Rd,C4}$ ($R^2 = 0.23$), sf_{Rd} ($R^2 = 0.16$) and f_{Ci} ($R^2 = 0.14$). All four parameters show a negative correlation and they explain most of the variance in ΔNLA . A list of all R and R^2 values can be found in Tables S3 and S4. Parameter $s\Delta S_{Jm}$ describes the acclimation of photosynthesis, i.e., potential rate of electron transport J_{max} , to plant growth temperature. Parameters $sf_{Rd,C4}$ and sf_{Rd} also describe the acclimation to plant growth temperature, but for the dark respiration of C4 and C3 plants, respectively. Finally, the fourth parameter f_{Ci} describes the reaction of the stomata to CO₂ (fraction of ambient to intercellular CO₂), that is which stomatal internal CO₂ concentration they maintain relative to the ambient CO₂ concentration. Our results thus indicate that most of the uncertainty in ΔNLA arises from acclimation to either leaf growth temperature or ambient CO₂.

[18] A time series plot of NLA is presented in Figure 3 for both the prior and posterior cases, showing in each case and for each simulation year the 5th, 50th and 95th percentiles of NLA. The curve of the 95th percentile is nearly the same for both cases, indicating that the use of the prior and posterior parameter values results in the same upper constraint for NLA. A large reduction in the uncertainty is achieved almost entirely within the lower part of the distribution of NLA (less than the median) so that, incidentally, the curve of the 5th percentile in the posterior case is very close to the median of the prior case. We further find that most of the interannual variability, i.e., the phase and timing of the fluctuations of NLA, is little effected by changes in the parameters of BETHY, while the magnitude of NLA as well as the amplitude of the interannual variability are.

This has already been observed by Knorr [2000] for net primary productivity.

4. Conclusions

[19] We have presented a generic method for combining trait data with process models in order to constrain model parameter values. In our case, we have used plant trait data to constrain Farquhar *et al.*'s [1980] photosynthesis model, which is now the standard photosynthesis model used in terrestrial ecosystem and Earth system models. The Bayesian approach has allowed us to combine different sources of data at leaf level (e.g., observations of parameters and photosynthesis and respiration rates and stomatal conductance) and we have derived a consistent parametrization of 29 PFT independent and 12 PFT dependent parameters.

[20] Through this method, we were able to reduce posterior parameter uncertainties, which in turn led to a reduction in the uncertainty by more than a factor of two for two key diagnostics related to the climate-carbon cycle feedback: mean NLA (NLA) and NLA change due to climate change (ΔNLA). The posterior parameter values led to a good agreement between simulated global GPP and observation based estimates. Given that data bases on plant traits are increasingly being made available to the modelling community [Kattge *et al.*, 2011], this method should be used extensively to parameterize Earth system models.

[21] A sensitivity analysis has further revealed that most of the posterior variation in ΔNLA is associated with the variation of a few parameters associated with the acclimation of photosynthesis and dark respiration to plant growth temperature, or the response of leaf stomata to ambient CO₂ concentrations. If we wanted to further reduce uncertainties in simulated NLA by any substantial amount, we need to better understand acclimation processes to plant growth temperature and CO₂. Currently only very few terrestrial ecosystem models represent those processes.

[22] **Acknowledgments.** This work was supported by the QUEST programme of the Natural Environment Research Council, U.K.

[23] The Editor thanks the anonymous reviewer for their assistance in evaluating this paper.

References

- Beer, C., et al. (2010), Terrestrial gross carbon dioxide uptake: Global distribution and covariation with climate, *Science*, 329, 834–838.
- Bernacchi, C. J., L. E. Singsaas, C. Pimentel, A. R. Portis, and S. P. Long (2001), Improved temperature response functions for models of Rubiscolimited photosynthesis, *Plant Cell Environ.*, 24, 253–259.
- Braswell, B. H., W. J. Sacks, E. Linder, and D. S. Schimel (2005), Estimating diurnal to annual ecosystem parameters by synthesis of a carbon flux model with eddy covariance net ecosystem exchange observations, *Global Change Biol.*, 11, 335–355.
- Collatz, G. J., M. Ribas-Carbo, and J. A. Berry (1992), A coupled photosynthesis-stomatal conductance model for leaves of C₄ plants, *Aust. J. Plant Physiol.*, 19, 519–538.
- Cramer, W., D. W. Kicklighter, A. Bondeau, B. Moore, C. Churkina, B. Nemry, A. Ruimy, and A. L. Schloss (1999), Comparing global models of terrestrial net primary productivity (NPP): Overview and key results, *Global Change Biol.*, 5, 1–15.
- Farquhar, G. D., S. von Caemmerer, and J. A. Berry (1980), A biochemical model of photosynthetic CO₂ assimilation in leaves of C₃ species, *Planta*, 149, 78–90.
- Friedlingstein, P., et al. (2006), Climate-carbon cycle feedback analysis: Results from the C4MIP model intercomparison, *J. Clim.*, 19, 3337–3353.
- Intergovernmental Panel on Climate Change (2001), *Special Report on Emissions Scenarios*, edited by N. Nakicenovic and R. Swart, Cambridge Univ. Press, Cambridge, U. K.

- Kattge, J., and W. Knorr (2007), The temperature dependence of photosynthetic capacity in a photosynthesis model acclimates to plant growth temperature: A re-analysis of data from 36 species, *Plant Cell Environ.*, *30*, 1176–1190.
- Kattge, J., W. Knorr, T. Raddatz and C. Wirth (2009), Quantifying photosynthetic capacity and nitrogen use efficiency for global-scale terrestrial ecosystem models, *Global Change Biol.*, *15*, 976–991.
- Kattge, J., et al. (2011), TRY—A global database of plant traits, *Global Change Biol.*, in press.
- Knorr, W. (2000), Annual and interannual CO₂ exchanges of the terrestrial biosphere: Process-based simulations and uncertainties, *Global Ecol. Biogeogr.*, *9*, 225–252.
- Knorr, W., and M. Heimann (2001), Uncertainties in global terrestrial biosphere modeling: 1. A comprehensive sensitivity analysis with a new photosynthesis and energy balance scheme, *Global Biogeochem. Cycles*, *15*, 207–225.
- Knorr, W., and J. Kattge (2005), Inversion of terrestrial ecosystem model parameter values against eddy covariance measurements by Monte Carlo sampling, *Global Change Biol.*, *11*, 1333–1351.
- Medlyn, B. E., et al. (1999), Effects of elevated CO₂ on photosynthesis in European forest species: A meta-analysis of model parameters, *Plant Cell Environ.*, *22*, 1475–1495.
- Rayner, P. J., M. Scholze, W. Knorr, T. Kaminski, R. Giering, and H. Widmann (2005), Two decades of terrestrial carbon fluxes from a carbon cycle data assimilation system (CCDAS), *Global Biogeochem. Cycles*, *19*, GB2026, doi:10.1029/2004GB002254.
- Santaren, D., P. Peylin, N. Viovy, and P. Ciais (2007), Optimizing a process-based ecosystem model with eddy-covariance flux measurements: A pine forest in southern France, *Global Biogeochem. Cycles*, *21*, GB2013, doi:10.1029/2006GB002834.
- Tjoelker, M. G., J. Oleksyn, and P. B. Reich (2001), Modelling respiration of vegetation: Evidence for a general temperature-dependent Q₁₀, *Global Change Biol.*, *7*, 223–230.
- von Caemmerer, S. (2000), Biochemical models of leaf photosynthesis, CSIRO, Canberra, ACT.
- Wang, Y. P., R. Leuning, H. A. Cleugh, and P. A. Coppin (2001), Parameter estimation in surface exchange models using nonlinear inversion: How many parameters can we estimate and which measurements are most useful?, *Global Change Biol.*, *7*, 495–510.
- Wullschlegel, S. D. (1993), Biochemical limitations to carbon assimilation in C₃ plants—A retrospective analysis of the A/Ci curves from 109 species, *J. Exp. Bot.*, *44*, 907–920.
- Yeoh, H. H., M. R. Badger, and L. Watson (1981), Variations in kinetic properties of ribulose-1, 5-bisphosphate carboxylases among plants, *Plant Physiol.*, *67*, 1151–1155.
- Zachle, S., S. Sitch, B. Smith, and F. Hatterman (2005), Effects of parameter uncertainties on the modeling of terrestrial biosphere dynamics, *Global Biogeochem. Cycles*, *19*, GB3020, doi:10.1029/2004GB002395.

J. Kattge, Max-Planck Institute for Biogeochemistry, Hans-Knöll-Str. 10, D-07745 Jena, Germany.

W. Knorr, M. Scholze, and T. Ziehn, Department of Earth Sciences, University of Bristol, Wills Memorial Building, Queen's Road, Bristol BS8 1RJ, UK. (tilo.ziehn@bristol.ac.uk)