Biogeosciences
Discussions

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Interactive comment on "Optimal Inverse Estimation of Ecosystem Parameters from Observations of Carbon and Energy Fluxes" *by* Debsunder Dutta et al.

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MAIN COMMENTS

The article presents a methodology to estimate parameters of a land-surface carbon and energy balance model (SCOPE) through a Bayesian non-linear inversion framework. First, the biochemical model of photosynthesis is modified to resemble the model implemented in the land-surface model CLM4.5. Then, the values of three important parameters: Vc,max, BBslope (the slope of the empirical function relating net assimilation to stomatal conductance) and LAI are computed for one growing season for three locations characterized by different vegetation types, a C4 crop, a C3 deciduous forest and a C3 evergreen forest. The methodology leads to estimate the seasonality

of the analyzed parameters (Fig. 9, 14 and 18) and improve model performance in reproducing carbon and energy fluxes (Fig. 12 and 16).

The article is generally well written, although with a large number of imprecisions (see detailed comments). From my evaluation the technical aspects of the inversion algorithm to estimate the parameters are rigorously implemented. However I have a number of concerns which are detailed in the major comments below.

(i) The algorithm of the Bayesian inversion framework is designed to provide robust numerical results and optimize the model parameters to reduce the mismatch between observations and simulations. However, the same results are likely less meaningful from a plant physiological point of view. This is important given the premises of the authors in giving a physiological interpretation of the parameters (Page 2, LL 7-9). When I see (a) Vc,max changing from less than 10 to 80 throughout the growing season (Fig. 9 and 14), (b) LAI decreasing from 5-6 to less than 4 in the second part of the growing season for a crop, which is expected, at the very least, to maintain the same LAI until harvest (Fig. 9), or (c) a threefold variability in BBslope, I tend to think, there is a considerable adjustment of model structural issues rather than an estimation of meaningful ecosystem parameters. This is hinted by the authors when they say that they do not include evaporation from interception or have a simplified soil evaporation (Page 20, LL 2-4). Surely, Vc,max or photosynthetic capacity have been observed to change seasonally even considerably in a single tree (e.g., Wilson et al 2001; Misson et al 2006; Bauerle et al 2012; Wu et al 2017) but not in a range that cover almost the entire variability of Vc,max globally (Kattge et al 2009). What would be the physiological explanation for such a variation in Vc,max? The seasonality of leaf nitrogen content is surely much less pronounced. I think what we see in the seasonality of parameters is largely a compensation of model structural inadequacy (e.g., the jumps in correspondence to major rainfall events) and only partially a real seasonality. Better constraints should be places on the potential range of the parameters. Furthermore, some of these "parameter" as the seasonality of LAI could be tested against ground

or remote sensing observations to support or disprove the values obtained in the optimization. It is also not surprising that model results are improved (even though it is not clear how much, since R2 results with the non-optimized model are not reported) since now the parameter space is significantly larger, being parameters allowed to vary seasonally.

(ii) A major issue is also the use of a single year for the three locations. In this way, the robustness of such estimates across different years remain untested. In my view, an important test, would be to use the constant and seasonal parameters over few other years and see if the prediction are better in the case of seasonally variable parameters. Saying that they are better when they are optimized is completely expected and trivial. Finally, I am glad the author consider uncertainty in the flux-tower data (Sε), which is a very important aspect given the considerable uncertainties in flux-tower observations, however, how they do (Page 16, Line 2-3) is not very clear nor justified.

(iii) I also have doubts about the overall novelty of the study. Several other studies have been published using Bayesian approaches to parameter estimation with inverse methods in ecosystem or land-surface models (e.g., Mackay et al 2012, Xu et al 2006; Wu et al 2009; Wolf et al 2006). For instance, the authors do a remarkable job in highlighting the subtle differences of their work with respect to Wolf et al 2006 (Page 3, LL 15-21). Surely, in this article, the model is different, the optimized parameters are different and the inversion methodology has some peculiarity but overall the idea and scope is not much dissimilar from the ones of previous studies. If the novelty is on technical aspects of the methodology, then "Biogeosciences" may not be the most appropriate venue.

(iv) Finally, some of the presented material is redundant. There is an entire manuscript part in comparing new and old implementations of the biochemical model of photosynthesis (Section 2.3 Fig. 2, 3, 4 and 5), which is just relevant for the SCOPE model users, since it is quite obvious that if one substitutes temperature functions in the biochemical photosynthesis module, he/she might obtain different results. These type of

analyses are carried out by any model developer all the time, without the necessity to write 5 pages of peer-reviewed paper about it. Figure 11 is also very technical and I think it would be more appropriate for an appendix or supplementary material than for a main text. The results described for the three sites are also separated and many explanatory sentences are repeated. Their presentation can be largely streamlined, combining Figure 8, 13 and 17, Figure 9, 14 and 18, and Figure 10, 15 and 19 and removing the repetitive parts, highlighting differences among the case studies, rather than iterating the overall result presentation.

DETAILED COMMENTS

Page 2 LL 5. See also Wramneby et al 2008; Pappas et al 2013.

Page 2 LL 18-19. Which model do you refer to? LSM, Ecosystem/Vegetation models or the biochemical models of photosynthesis? The first they also require shortwave radiation and precipitation as input and information about soil depth and properties, at the very least.

Page 2. LL 26. Rate-limiting, strictly speaking, refers only to Jmax not Rd.

Page 2. LL 33-34. LAI in most of Terrestrial Biosphere Models is a prognostic variable not a parameter. As you correctly wrote in Page 3, LL 13-14. I think, this needs to be stated here.

Page 3. LL 2. LAI can be also estimated from destructive observations.

Page 3. LL 12 and Page 4 LL 12. SCOPE can model "spectrally resolved" radiation, but it remains unclear throughout the manuscript how many wavebands and which ones are considered?

Page 3. LL 22 See also Mackay et al 2012.

Page 3. LL 25. I would write "often the associated computational costs..."

Page 3. LL 26-31. While I completely agree that modeling SIF and comparing SIF with

observations is very important, since SIF is not explicitly used in this manuscript, such a long paragraph in the introduction, deviates from the main focus of the article.

Page 4. LL 26-28. So, in the end, how many prognostic temperatures do you resolve in the system? E.g., 2 temperatures for each layer for how many layers?

Page 4. LL 28. Since you brought this up and this is not an easy problem to solve. Are iterations repeated until convergence? Which tolerance is used for convergence? If not, how many iterations are used?

Page 5. LL 10-16. I found this part explaining differences with CLM4.5 at least awkward. As a reader I want to know what you do now, not what was different from CLM4.5 in the previous model version.

Page 5. LL 20-21. Please move to an earlier part of the section the explanation of what CLM is.

Page 6. LL 1. There is no mention of the parameter "intrinsic quantum use efficiency" or "quantum yield of photosystem II" depending how it is expressed. While it is considered constant by most biochemical models, this could also exhibit some variability (e.g., Skillman 2008) and could have been integrated in the optimization framework.

Page 6. LL 4-5. As before, please delete the second part of the sentence "in the earlier SCOPE version it was implemented as potential ETR x CO2 per electron", this is not relevant here.

Page 6. LL 15-20. Cs is not defined, but it must be the CO2 concentration on the leaf-surface, otherwise a leaf boundary layer resistance would be necessary in Eq. (1) and (2).

Page 6. LL 26. Iterative methods to solve the $A - Ci - gs$ system were already included in ecohydrological models, (e.g., Ivanov et al 2008 and other land-surface models before that).

Page 7. LL 1. This is repetitive, it has been already stated a few times.

Page 7, LL 6-7 and Figure 1, Caption. It is not clear what $\pm\sigma$ variability means. It is the variability in the parameters of the temperature functions, how σ is defined? Is the standard deviation of which parameter? What data from Leuning 2002 are considered/used for the plots? Are the temperature parameters rather than data taken from Leuning, 2002?

Page 7. Line 16. The two sites are not defined yet, their description is arriving much later in the manuscript, while it should be made upfront.

Page 8. Line 5, Figure 5 and Page 11 Line 4-6. Which version has been calibrated to the data? It is not surprising that the newer implementation is closer to observations, if Vc,max or other parameters have been optimized for the newer version. For instance, in Figure 5b you could likely adjust the value of Vc,max to obtain an opposite behavior, where the old model is unbiased and the new one is.

Page 8. Line 9-10 and Figure 3 and 4 caption. I do not think you are showing any result for the Missouri Ozark site or Nebraska-Mead-1, you just use the meteorological forcing and C3 vegetation type derived for these sites to run the two version of the biochemical model and make a comparison. Strictly speaking you could have done a test varying temperature, VPD, and PAR for C3 and C4 vegetation without referring to any specific site. However, I do not find this part generally insightful for a journal article.

Page 13. Line 4. The Jacobian depends on the linearization point, X_l, which is somehow approximated for any optimization window. This is discussed later but maybe it should be stated here already.

Page 13. Line 14-15. It is fine to have a more in-depth treatment in the appendix, but at least you need to define the terms, Ki (the Jaobian matrix) is never defined at this stage of the article.

Page 14, Figure 6, and also Page 22, LL 5-6. Some of the derivative values are

a bit surprising. Why LE is decreasing with increasing LAI? Is due to self-shading effects? This is generally counterintuitive. Even more difficult to understand is why LE decreases with increasing Vc,max. Higher photosynthesis should lead to higher stomatal conductance and thus higher LE, especially in a model like SCOPE. These unexpected behaviors need justification.

Page 15. Figure 7 caption. You need to specify what is "m" and what is intended here for ΔX. Plus, it should be better stated what the measurement vector refers to, since the derivative must be computed with model outputs.

Page 16. Line 2-3. The observational error matrix S_ε is quite important given the general uncertainty of flux-tower observations. However, from such a brief description "using noise standard deviation as 10% of observations" is not clear how this is computed. Does it mean that you assume an uncertainty of 10%? This is likely quite a low number in the context of flux-tower observations (e.g., Leuning et al 2012).

Page 16. Line 5. Which iteration step? The current one? This is relevant since K depends on where it is computed.

Page 16. Line 6-7. I am not sure I can see very well the concatenation between observations Y and modeled values F(X) in Figure 7. I just see ΔY.

Page 16. Line 20-22. I agree with the authors that 3-days sounds as a reasonable length for separating the time scales of parameter variability and meteorological forcing. But, what does it happen if you modify the time window and instead of 3 days you select 7 days or 15 days? Do you get similar seasonality of parameters? This is a test, which could be relevant in the scope of this article.

Page 16. Line 24. I do not find where this is mentioned in Section 5.

Page 17. Equation (17). The subscript "jj" is undefined.

Page 18. Figure 8. Did you see that incoming shortwave radiation is reconstructed and actually almost equal for the first 60 days? Afterwards, fortunately, you do not use this

period because it is not in the growing season, but such type of artifacts, which are frequent in Fluxnet data, could jeopardize your procedure. This may need a mention.

Page 18. Line 8. Why did you select a single year? I think it would be rather important to see how seasonality of parameters is retrieved in different years.

Page 19. Line 8-9, Please provide references for such changes in BBslope, LAI and Vc,max if they are found to be reasonable, which I do not think it is the case for BBslope and Vc,max

Page 20. Line 12 and captions of Figure 10 and also Figure 15 and Figure 19. If it is a "correlation coefficient", why the symbol r2 is used, this is typically reserved for the "coefficient of determination", and not for the correlation coefficient, which is typically indicated by r.

Page 21. Figure 11. The x-label with the indexes is not defined in the figure caption but only in the main text.

Page 22. LL 7 and LL 10 and Figure 12 caption. How much is it this "net improvement"? The value of R2 for the previous parameter set is not reported, values are only reported for the optimized model.

Page 23. LL 12. It is quite well-known that the growing season is longer for a deciduous forest than for a crop. I would suggest eliminating "we find".

Page 24, LL 13 and Page 29, LL 6-7. What could justify a threefold change of BBslope in a single growing season? This is theoretically an intrinsic property of the stomatal regulation, I can see how can change during leaf development (very first part of the growing season) or if water stress occur, but I do not see what can justify such a large variability throughout the entire season.

Page 25. LL 13-16. The value of R2 for the previous parameter set is not reported, values are only reported for the optimized model. How much the results were improved remains unverifiable, although clear from Figure 16.

Page 27. LL 2-6. Please consider that at Niwot Ridge snow-cover is affecting energy exchange and potentially GPP for a large fraction of the year. It is true that you focus only in the snow free-period, but this confounding element needs to be stated somewhere.

Page 27. LL 10. The constraint on LAI from observation is a very good addition to the modeling exercise, I would have liked to see this type of constraints placed also for other sites, or parameters, whenever available.

Page 29. LL 16 and Page 30 LL 4-5. I am sorry, but I am thinking you mostly retrieve "model parameters" and not "ecosystem parameters", and I also tend to think you are "overfitting" the SCOPE model rather than constraining it. The advantage of using seasonality of parameters for predictive simulations (e.g., in other years or other conditions) remain to be tested.

Page 29. LL 22. Yes, LAI and $V_{c,max}$ have seasonal variability but for $V_{c,max}$ unlikely in the order of magnitude that is presented here.

Page 29. LL 27-30. While interesting the discussion on SIF is out of place, since SIF is not used or treated in this article.

Page 30. LL 16. Optimality approaches (e.g., Medlyn et al 2011, Katul et al 2010) do not typically comprise soil-moisture dependences, which therefore need to be included as additional parameterizations.

Page 30. LL 18. Rather than "better solution", I would say it can provide "optimized model parameters."

Page 30. LL 19-25. All this paragraph is emphasizing the technical aspects of the "optimal inverse estimation of the parameters", I am wondering if this is the most effective way of concluding the manuscript.

Page 31. LL 7-8. This sentence is quite repetitive.

Page 34. LL 9. I would suggest to write "will allow us".

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