

Reply to anonymous referee 1:

We would like to thank the referee for their review of this manuscript and their constructive comments. Below is a response to each comment (the referee's comments have been included in italics).

*"if one assumes a Gaussian prior that extends into negative values when these make no physical sense, and a negative assumption is provided by the scheme, we need to interpret this as a consistent solution (consistent with the model as it stands, and with the prior description)."*

The negative assumption is a solution however it is not useful in this context since it breaks the physical laws. And it is a solution to an ill-posed problem because we know that for the real problem a negative value is not a viable solution. But we agree that it is a consistent solution with the current model formulation together with the prior and data information. Still, we can learn from this:

- If, for a certain process in the model, the posterior parameter value takes on an unrealistic value (either non-physical or even physically correct but non-sensible, e.g. a Q10 value of >10) this may hint to an incorrect model formulation or even a missing process in the description of the model. The occurrence of unrealistic posterior parameter values therefore always requires an analysis of the course of the optimisation and the residuals. One way to resolve this could be further model development and include missing processes in the model formulation. But this is not always feasible and therefore we use the current model formulation with parameter transformations to ensure physically meaningful parameter values.

- A process-based terrestrial ecosystem model contains many non-linear functional relationships and large number of parameters such that the parameter space is a highly complex multi-dimensional space. In a strictly mathematical sense it could well be the case that an optimum point is found at a non-physical value if the definition intervals of the respective parameters are not restricted (through either parameter transformations or constrained optimisation).

*"I think that instead of looking at the MAP value of a particular parameter, we need to address the whole distribution, and maybe decide that if the prior has a very large amount of weight in the non-physical space, it should be narrowed or modified."*

In fact, we do look at the distribution and not only the posterior optimum value (or MAP). But this does not circumvent the fact that when assuming a Gaussian PDF (which is the case in our Bayesian parameter estimation framework) parameter values are not restricted to a certain interval. The parameter transformations transform the whole PDF such that the relative weight of each parameter is not changed. We could narrow the uncertainty but we want it to be realistic and as little is known about some of the parameters, we would like to start with a larger, realistic uncertainty. We have clarified this in the manuscript.

*“The authors pursue some parameter space limitation strategies. The first one is the addition of an extra “penalty constraint”. This approach has problems, as it basically changes the prior term to something different. The resulting cost function is also dependent on a number of parameters (D18,  $\mu_{18}$  in the paper, Eq. 10). These choices have implications (you are solving a different problem after all), which the authors do not address (despite the fact that the method didn’t work!)”*

When we limit the parameter space, we actually do change the optimisation problem. So, yes, the penalty term experiment optimises a slightly different problem, but so does the parameter transformation experiments. The constrained experiment uses the same problem but the search space is restricted. We chose D18 to be on the same order of magnitude as the cost function at the minimum of previous experiments and  $\mu_{18}$  had to be positive but we did not want to use 2 as we use the 2<sup>nd</sup> derivative to calculate posterior uncertainties.

*“The authors do not address why the optimiser boundary experiments fail to converge. It would be interesting to know the reasons behind their results, as it’s the most logical way for users to impose constraints (for example, how does the bounded space relate to the prior pdf?)”*

For the constrained experiments, four out of the five optimisations failed to converge because of internal overflow problems within the optimiser and the fifth one (started from the default prior parameter values) stopped because of reaching the maximum number of iterations (5000, which is about 10 times more than the average number of iterations for the parameter transformation experiments). Also, for this optimisation, the selected parameters for bounding were exactly at their limits, which, at least in the case of 0 for a beta parameter, does not make sense.

The constrained approach produces a prior of Gaussian shape inside the bounds and a zero probability outside the bounds.

*“The transformations are useful, but their form (the double bounded transformation) is not included! This is a major oversight! Please include the transformations you used in the paper (was it a simple linear transformation, or a more complicate transformation? We don’t know).”*

We have included in the manuscript the equations explaining how the transformations are made.

*“Additionally, why not calculate the uncertainties in transformed space and transform back e.g. the 5-95% CI? This should hopefully result in uncertainties that are now bounded, and thus more realistic.”*

In fact, that is our normal procedure to calculate posterior parameter uncertainties. We have included the one-sigma confidence interval in physical space in Table 3 in the manuscript.

*“Finally, Section 2.2 should be shortened, as most details are of little relevance to this study. Figure 2 is unnecessary. Figs 6 is superficially discussed, and Fig 7 should be better presented: as it is, it looks like an optometrists test!”*

As the second reviewer has asked for extra details in section 2.2, we have decided not to shorten this section. Figure 2 has been removed from the manuscript as well as Fig. 7; we agree with the second reviewer that it does not add any new information. Figure 6 is now discussed in more detail.

*“Finally, a table with the prior extents would be useful (see comments above) to compare the boundaries of the parameter to the true extent of the prior.”*

We have included a table comparing the boundaries of the posterior parameter to the prior (see response above).