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Interactive comment on "Calibrating a wetland methane emission model with hierarchical modeling and adaptive MCMC" *by* Jouni Susiluoto et al.

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Editor comments

E1: The main paper must give the model name and version number (or other unique identifier) in the title.

A: The final paper contains the model name and version number in the title.

Anonymous Referee #1

The authors use a reduced order model representation of a complex numerical wet land methane model with adaptive MCMC to estimate posterior distributions of model

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parameters. Because wetland methane models are complex and surface CH4 emissions are small differences between large gross fluxes, this type of calibration exercise is difficult and potentially valuable.

The authors did a nice job describing their results, given their model setup and assumptions. At this point, however, several assumptions in the approach leave me unconvinced of the reasonableness of the results, which I describe below. Also, the underlying model has not been described in the literature, and citing “Raivonen et al. (2017)” is inappropriate, since it is apparently a paper in preparation.

A: We thank the Anonymous Referee #1 for her/his constructive critique and we address the points raised below. Here, we would like to point out that Raivonen et al. Is in public discussion in GMD, and therefore available for consultation. The list of references that we provide at the end of the article has the old reference to “in preparation” paper, which is unfortunate. Whe have added the link, https://www.geosci-model-dev-discuss.net/gmd-2017-52/ to the references.

Major comments

R1/1. It is unclear why you need to vary the peat depth in your optimization. You apparently have measurements of the depth (lines 22-23, page 4), so you ought to use that as a non-calibratable value in the model. The high sensitivity of your parameter calibration to the peat depth implies to me that some other factor must be important and not properly resolved in your underlying model (e.g., O2 profiles below the WT depth or rooting profiles). The argument on line 31, page 6 that it is more computationally expensive to run with a deeper peat depth is not sufficient to justify this approach.

A: Peat depth of a wetland is not constant and therefore using a measured value is not as straightforward as is suggested. The peat depth affects in sqHIMMELI both production and transport. The high sensitivity of the parameter tau_C_cato suggest, as discussed, that the total catotelm decomposition rate is relatively constant as it is positively correlated with peat depth.

We changed the model to include the full 4m deep peat layer, by increasing the thickness of the lowest layer, and mention that this value is not an absolute truth but is to be looked at together with the tau_C_cato parameter, because of the variability of peat depth at any given wetland site, and the heterogeneity of the site. In MCMC experiments, 500000 sequential simulations are often needed, and the posterior estimate improves with more simulations, so in our opinion computational efficiency does matter. If the model simulation takes five seconds longer to finish, we end up spending 29 days more on the simulations.

As both referees wondered about the changing discretization level numbers, We drop the part of the study looking into that, and only concentrate on a single experiment.

R1/2. Changing z_exu and Q10 on a yearly basis seems arbitrary. For Q10, I would expect much larger seasonal than interannual variations, yet you ignore that possibility. I think you need to explicitly describe the mechanisms you are proposing for the interannual variability of these parameters. The citation to Bergman et al 2000, who noticed change in Q10, "even within a single year", seems to bely your approach.

A: We could have added an additional model for the parameters Q10 and z_exu, but decided that a simpler approach serves us better here as we do not want to overfit the parameters. Bergman reports the following mid-July – late Sept. Q10-values for minerotrophic lawn, which is closest to the Siikaneva site (Laine et al.) whose data is used in the manuscript: 5.9, 3.7, 8.4, 4.0, 7.1, 4.1, 7.0. This suggests that the seasonal variation can be quite irregular at such sites, and in such a situation we opt for the simplest description of the variation. We would like to note here, that for the calibration we feel it is enough to be convinced that there is variation, and the mechanisms are a research question to be tackled in a separate research project. However, we note that these mechanisms are discussed in e.g. (Davidson et al., 2006), and we add a short section about it to our text.

R1/3. Ignoring the temperature sensitivity of CH4 oxidation appear to be a flaw in

your approach. There is substantial evidence that this temperature dependence is even larger than that for CH4 production. Further, since the net surface emission is a small balance of production and oxidation rates, and you explicitly account for the CH4 production temperature sensitivity (eq. (5)), not including Delta(E_R) in your equation (7) seems unreasonable. a. This concern propagates to the last sentence in your abstract. Oxidation often strongly affects the net CH4 emission, which is the measurement you are using to calibrate. If parameters affecting oxidation are 'not identifiable', then it seems unlikely that the production parameters are reasonable.

A: We re-performed the simulations and added Delta(E_R) in the parameters to be optimized. We add the relevant parts to the discussion and reformulate the abstract to reflect the changes. We also added the Delta_E_oxid parameter to the optimization, that regulates the temperature dependence of oxidation of the parameters. It is true that the oxidation and production terms are correlated, and this is something to beb expected. Nonetheless, also information regarding their correlation is important and as such scientifically valuable, as their mutual relationship may still be well defined.

R1/4. On line 21 of page 7, you state that V_R0 affects the rate of temperature dependent HR, but the T dependency is actually governed by Delta(E_R) which is not used in the calibration (Table 2). In general, it is unclear in your section 3.4 how the CH4 production occurs and its relationship with heterotrophic respiration.

A: This is correct, the shape of the temperature response is governed by Delta(E_R). We clarify the functions of the parameters regarding the HR in the text and also discuss the role of Delta(E_R) that was added in the new simulations.

R1/5. In section 4.1, you say the model was linearized, but you did not show whether such a linearization is a reasonable approach. Please provide a quantitative evaluation of how appropriate this linearization

A: This was an error in the text. The linearization was done for the posterior probability density function and not to the model, and was used only in estimating the initial

proposal covariance for MCMC. In the new simulations we do not use this method and hence this part of the text is dropped.

R1/6. Lines 22-25, page 9: Having to restart the model on January 1 of each year because realistic column gas concentrations were otherwise not predicted is a red flag for a problem in the model. The model should be able to run continuously without interruption. If this is a real problem in the model, you should rectify it. Once rectified and described in the paper, restarting each year for computational efficiency and parallelization is reasonable.

A: The concentrations are realistic and stable and the reason for the restarting is just the optimization algorithm, which allows using separate parallel simulations for different years. We wanted the peat column gas concentrations of any year in the optimizations to be in the regime of the parameters to be optimized, but since the variations are small, we actually believe, that this is more than enough. In the end the model will of course be run linearily in a single simulation, and this can be done already now with only trivial changes required to the model.

R1/7. Section 4.2.4 seems to apply that your objective function is only based on annual values, but the text implies that you use the annual values to linearize the model, and then perform the parameter calibration with observed daily CH4 emissions. Please clarify.

A: The annual component was dropped from the new simulations as they had no practical effect to the posterior. The text is updated accordingly.

Smaller comments:

R1/8. Methane is the second most important anthropogenic GHG for warming (don't forget water vapor).

A: This is now mentioned in the text.

R1/9. You describe annual calibration in they abstract, but not the fact that you used a

ROM and then daily fluxes for calibration (as far as I can tell). This approach should be described in the abstract.

A: The annual values were dropped, see R1/7. Also, a reduced order model was not used, and in the updated work it is not used even for covariance estimation.

R1/10. Line 13-15, page 2: cite recent methane model inter-comparisons here: Melton et al., Bohn et al.

A: Citations were added to text.

R1/11. Your assertion (lines 33-34, page 2 to line 4, page 3) that flawed physics representations, numerical errors, and coding errors are good reasons to calibrate a model is shocking. Calibrating a poorly constructed model is a cardinal sin of modeling, although it is regularly done. I think you might re-think the organization of this paragraph.

A: We clarify the text. However, we would like to point out that even excellent models require calibration. Model parameter optimization is effectively inverse modeling, which can improve predictive performance, reveal bottlenecks, and in the best cases provide information for analyzing the physical system. This being said, it is fully true that blindly done model calibration can lead to strange results and a worse model. We reorganize the section to better clarify our views on the topic. We also mention that proper description of the physics is important for the calibration exercise to make sense.

R1/12. Line 5, page 3: Possibly the most mechanistic and realistic terrestrial CH4 model available today is ecosys (Grant, 2002), which you should cite.

A: Citation has been added to the text.

R1/13. Line 8, page 3: define 'multi modality'

A: The text has been clarified in regard to this.

R1/14. Your figures are cited out of order in the text (e.g., figure 11 cited just after figure 2).

A: The figures are now in order.

R1/15. Line 27, page 12: do you mean ‘inter-annual variability’ instead of ‘annual variability’?

A: Yes, fixed.

R1/16. Line 9, page 12: there is no figure 6g.

A: Should have been 6 (b), fixed

R1/17. Does the model calculate the peat temperature? It is not clear from your description which T you are using to estimate your temperature sensitivity. Air T?

A: The model uses any soil temperatures that it is given. In this work we used everywhere measured soil temperatures. We clarify this point further.

R1/18. What happened to a discussion of figure 10?

A: A short discussion was left out and is now added.

R1/19. Where did the NPP come from? Describe in Methods.

A: This is explained in the appendix, but is clarified in the main text now.

Anonymous Referee #2

The objective of this paper is to use observed carbon flux time series in order to optimize parameters of a peatland carbon flux model. In general, this is a timely and important work. However, I found several serious issues with this manuscript including potential flaws in the method that does not allow a publication in the present form.

Please, indicate in abstract and introduction, what is the overall objective of this model e.g. in future applications? Do you want to apply it exclusively for this one peat site and for which question? Do you want to apply it on a continental to global scale, e.g. as part of a land surface scheme? In the latter case, several model assumptions are not useful (effective peat depth, C pool-independent decomposition flux), and a lot of work

on parameter optimization seems to be questionable when only data from one specific site is used.

A: We thank Anonymous Referee #2 for his/her valuable comments.

The HIMMELI model will be used in both stand-alone configurations and as parts of land surface components of regional and global models. We do not intend that the parameter optimization work here would be relevant to any wetland site – rather we look at within-site variation of parameters. The model assumption-related problems are addressed in the points below. We also further clarify the objectives of the research in the abstract and the introduction.

Major comments to sqHIMMELI assumptions:

R2/1 In both aerobic and anaerobic cases, organic matter decay seems to be a constant parameter not depending on substrate availability. When peat depth would have been set constant to the observed site-level value, then this could be valid for the specific site but then we do not learn anything from the parameter optimization procedure for a generally applicable dynamic model.

A: In the model, the organic matter decay (anoxic peat decomposition, Eq. A6) is not a constant parameter but depends also on the amount of peat and its temperature. And of course e.g. oxygen concentration affects the decay rates. We would like to point out for clarity that Eq. 5 in itself does not determine the reaction rate. In addition to moving appendix A into main text (as requesed in referee comment R2/15), we clarify in the text this point.

We re-performed the simulations with a 4m total peat column, which reflects our knowledge of the peat depth at the Siikaneva site (Rinne et al. 2007). Anaerobic respiration of exudates on the other hand does not depend on the peat column thickness. We clarify this in the text.

As peatlands differ widely from site to site, naturally these different types of wetlands

have different parameters controlling the organic matter decay. In the manuscript we look at the decay rates for a single site and as such the parameter values are not directly generalizable everywhere. However, we believe that we could, by looking at data from other sites, calibrate the model for various types of wetlands with e.g. hierarchical Bayesian methods, and this would make it possible to e.g. use the model with land surface sceme. This is work still waiting to be done and beyond the scope of this manuscript.

R2/2 Effective peat depth: This assumption makes no sense at all. Peat depth should be a constant value corresponding to the site observation. See below for related flaws in eq 5.

A: We have changed the peat depth to 4m that roughly represents the peat depth in Siikaneva. We no longer speak about effective peat depth in the manuscript. The different simulations now refer to how deep the fine discretization of the peat column goes. Please see also the answer to R1/1.

R2/3 A2 Anaerobic respiration producing CH4: It seems from eq. A5-A8 that you apply a CH4:CO2 ratio of 1:1 for anaerobic decomposition of root exudates. If so, please make this statement explicit and cite experimental literature showing this ratio.

A: We initially optimized the ratio along with other parameters, but due to covariability with the z_exu parameter without CO2 data, we left this parameter out as only z_exu or the ratio-determining parameter could be determined, and for the first iteration we chose 1:3. However, with CO2 flux data, we are able to constrain the parameter, and therefore we add it to the optimization and to the discussion.We now use data from (Nilsson & Öquist) to set the prior values and explicitely state the final ratios.

R2/4 In section 3 it is also fully unclear if you consider anaerobic CO2 production or not.

A: We do. This is now also clarified in the text.

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R2/5 Eq. 5: is tau(cato) the mean residence time at 273.15 K? The unit (y) in Tab 3 is not correct because in eq. 5 you do not multiply with a Cpool.

A: Equation 5 just describes a rate parameter, equation A6 is the actual peat decomposition. When tau has the units of time, A6 then has the time in the denominator which is correct.

R2/6 I expect the Finland peat being frozen with snowpack above over long time periods of the year. What are the effects of <273K soil temperature on aerobic and anaerobic decomposition? What are the effects of soil ice on gas transport and what are the effects of snow on gas transport?

A: Ice and snow slow diffusion of gases into the atmosphere, but this has not been so far implemented in HIMMELI, except for some very preliminary and simple efforts. We tried increasing the resistance of the top soil layer when top soil temperature fell under 0 C but this did not improve the fit / change the results enough for that the change would have been reasonable to keep. We have hence not included descriptions for processes such as diffusion through snow, or release of accumulated gas bubbles under ice in spring time as described by e.g. Mastepanov et al. (2013), Sriskantharajah et al. (2012) – this will be very interesting and will hopefully be done at a later stage.

R2/7 Please include in results and discussions the exudate pool values.

A: We add the exudate pool values and briefly discuss them.

R2/8 Peat depth: Prescribing an effective peat depth will hinder any application of that model in larger dynamic models, such as land surface schemes or DGVMs. Peat depth is no parameter there that you can prescribe but included into the mass balance equations. If you define an effective peat depth then this would mean that you either introduce a fully recalcitrant carbon pool (case peat depth > effective peat) or that you "produce" CH4 and CO2 from non-existing carbon (case peat depth < effective peat depth). That is not a valid and also not useful model assumption.

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A: We are not modeling for peat depth changes in this model so far. Of course, the decay in m yˆ-1 can be calculated in a straightforward way, but since we don't know the speed of new peat formation we don't know the change of the peat column in time. This work will be done later. We have changed the peat column depth to reflect the real depth. We have dropped the notion of effective peat depth.

Major comments on the parameter optimization:

R2/9 Tab 5: What is the reason for not including these parameters into MCMC optimization? I generally think that the information content in the data is far too low for an optimization of all model parameters, hence a selection will be useful. However, we need good reasons for such selection, either based on theory or based on a previous sensitivity analysis.

A: The selection was based on a previous preliminary analysis. This is now mentioned in the text. In practice not fixing some of the parameters may lead to ending up in local minima that are unrealistic. However, more importanly, parameters are interlinked via the model processes and in order to constrain the parameters determining the most important processes we fix some of the less important ones. We now explain for all non-included parameters why they have not been included.

R2/10 I assume there is additional CO2 flux data available at the site. It is totally unclear why this data has not been used for constraining in addition to CH4 parameters such as decomposition and transport parameters as well as oxidation parameters

A: We have re-performed the simulations also utilizing CO2 flux data. The setup description, results, and the discussion have been updated.

R2/11 parameter values cannot be transferred to other similar models and even not to HIMMELI because of the peat depth parameter and because of important differences in model formulations: root depth distribution, decomposition parameterization, etc. What is the scientific value of the paper then? Do you plan to use this model version in

future studies and not the HIMMELI model?

A: We plan to use both sqHIMMELI and HIMMELI in future studies. The decomposition parameterization is not part of the HIMMELI model but it can still be used as a source of the anaerobic respiration, which is an input variable for HIMMELI. We believe that the results are transferrable to other models variably: the optimal values of course are not so straightforward, but correlations of the processes more so. HIMMELI is a model more suitable for integration in land surface schemes, whereas sqHIMMELI is a version of the model more designed to be used in stand-alone experiments and settings such as MCMC studies. We will in future studies also integrate features from both model version's development into each other. What model version we use for future studies will depend on the research question at hand.

R2/12 section A4: I do not understand the sentence "Due to coding mistake, the fD,a and fD,w coefficients in the aforementioned equations were set to 0.1 for gases other than CH4 in this work." Why do you set both parameters to 0.1? With a huge pore volume in peat soils I would expect a value of 0.8 or 0.9. If that is a tuning parameter then you should optimize it. These parameters are also not listed in Tab 5. Instead they are part of Fig 2 and this seems to be a real flaw in the procedure?

A: This flaw has been fixed in the new simulations.

R2/13 For clarity, please put units on all parameters in tables and figures or when describing parameters in the text.

A: This has been done.

R2/14 I cannot understand the a posteriori optimized parameter values of tau_exu in the order of magnitude 0.00001 s (tab 3) when range is 3 to 30 days with a prior of 14 days (tab 2). From Fig 3 it seems there is a mistake in units in the table. I have similar problems with units of a posteriori V_0R which seems to be far too high. Zeta_exu seems to be with 0.5 also quite high and it would be good to see some comparison

to literature values if available in the discussion. tau(cato) ranges from 2000 to 20000 years (unit in tab 3 wrong however) depending on peat depth just because the model invalidly does not take the carbon pool into account for calculating the decomposition flux (eq. 5). Then of course, the deeper the peat the more C available the higher you need to have turnover time for the same flux. This is not a valid approach for a dynamic model.

A: For the units, we believe that Table 3 is correct: if tau_exu x 0.00001 = 10, then tau_exu = 10^6, which is around 11.6 days. Same is true for tau_cato and V_0R. The zeta_exu parameter is high because of a non-optimized another parameter f_methane in the model.That parameter value has been added to the optimization. We would like to note also that the decomposition flux is given by equation A6 – equation 5 gives just the reaction rate constant and if tau_cato has the units of years, the peat decomposition flux given by A6 becomes, integrated over the depth, moles per second per square meter. For the last sentence, we refer to replies to R2/1 and R2/5.

R2/15 A minor comment: I do not find it useful to have some methods description in the main text and some in appendix A but both relate so strong to each other that one understands it only when reading both together. Please move appendix A into main methods text.

A: We have moved the appendix A into the main methods text.

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