

Dear Referee,

Thank you for taking the time to read our manuscript and for giving good and useful comments. They helped us to see shortcomings in this work and taking your comments into account would improve it. Especially the aim of the model and the manuscript in general should indeed be better defined. Below we reply point-by-point to your comments. We hope you find the responses satisfactory and we can prepare and submit a revised version of this manuscript along the lines we suggest below.

A change that we suggest, not directly as a response to any Referee comment, is related to the model parameters. A set of parameter values that we use in the manuscript was taken from an optimization done using Markov chain Monte Carlo methods with observational CH<sub>4</sub> flux data from the Siikaneva peatland site, and we refer to Susiluoto et al. (2017, in prep.). The final results and a more exact description of the calibration work are now reported in Susiluoto et al. (2017, GMDD-2017-66). However, there were some major differences between the approaches used here and in the final version of Susiluoto et al., which led to some difference in the values. As the parameter values are not the main point of the present work and as the values here produce a good fit with observations, we suggest that we keep the current values for the revised manuscript. However, in the revised version we will not anymore refer to Susiluoto et al. but add in the Materials and Methods section the description of the optimization.

Referee comments are typed in italics. They are followed by our responses and suggestions of how we would revise the manuscript, as plain text and numbered referring to the comment number.

*In this paper, a methane submodel is proposed for use in a larger ecosystem C model. While this is a topic of interest to readers of the journal, this submodel has several key weaknesses that affect its acceptability for publication:*

*(1) It is driven by inputs for anaerobic respiration calculated as a first order function of peat C and root exudation derived from assumed vertical distributions of root mass in the anoxic part of the soil profile (Eq. 6). While I appreciate that anaerobic respiration is an input rather than an output of this model, it is nonetheless the key driver of CH<sub>4</sub> production, as noted in p. 14 and Fig. 11. Anaerobic respiration therefore needs to be explicitly simulated as part of any CH<sub>4</sub> model, rather than optimized for site conditions as done here, as it directly determines modelled CH<sub>4</sub> emissions. The determination of  $P_{max}$ ,  $R_{ref}$  and  $dW_{tol}$  (a poorly constrained term) in eqs. B2 and B3 is necessarily site-specific and detracts from model robustness. This optimization overlooks the possibility that anaerobic respiration can occur in wet soil above the water table. Model testing of anaerobic respiration could have been better constrained by including tests of modelled CO<sub>2</sub> fluxes with modelled CH<sub>4</sub> fluxes in Fig. 10.*

(1) Response:

We agree that simulation of anaerobic respiration is a significant, perhaps the most significant, component of a complete model of peatland CH<sub>4</sub> emissions. However, the target of our work was to produce a module that simulates only the transport and oxidation of CH<sub>4</sub>. The reason for this is that there are soil carbon models that simulate anoxic respiration and the interface to a CH<sub>4</sub> module would be through the respiration. Two examples of this kind of model environments are land surface models JSBACH and JULES. Therefore, we think that a CH<sub>4</sub> module that is driven with anoxic respiration is a justifiable modelling unit and in order to ensure its functionality for further use it is reasonable to analyze its sensitivity and performance independently.

The purpose of presenting the (already published) NPP model in the Appendix B is not to claim it is a general photosynthesis model for all the peatlands but, by contrast, to show that we

created as realistic NPP as possible for the model testing. The Siikaneva test was done to demonstrate that combined with realistic input, HIMMELI does output realistic CH<sub>4</sub> fluxes, which is not so evident if looking only at the mechanistic sensitivity tests. It is true that the parameter values for the NPP model are mainly from a study done at an oligotrophic fen, like Siikaneva. However, we think that in this model-data comparison it is not a downside to use a carbon input that corresponds to reality as closely as possible.

We also agree with the Referee that the choice of using water table depth (WTD) as a strict divider of the peat to oxic and anoxic parts is a simplification and as mentioned in Section 2. 'Key factors for CH<sub>4</sub> transport and oxidation', water-filled, anoxic sites can occur above it. In our opinion, however, it is uncertain to what extent the model estimate would be improved e.g., by assuming a certain volume of anoxic microsites in the peat above the WTD, which in practice would mean adding new unknown parameters. In any case, most of the peatlands have microtopography, hollows and hummocks, and even the observation-based site-level WTD is only an approximate value for the peatland, not to speak of a modelled WTD. On these grounds, we think this strict division to anoxic and oxic parts is, although being simple, a robust enough approach to be used in land-surface models.

Including modelled CO<sub>2</sub> fluxes into Fig. 10 is indeed a good suggestion.

(1) Suggested changes to the manuscript:

In Introduction, we will clarify the aim of HIMMELI and explain more clearly why simulation of anoxic respiration is not included in the model.

We will clarify the role of the Siikaneva test in the paper and, as suggested by another Referee, we will add a comparison of the model with data from another peatland site. This will be a test of how well the current parameterization fits to other peatland sites.

We will add discussion about how realistic is the strict division to oxic/anoxic parts of peat, on page 7, Section 3.1.2.

We will add CO<sub>2</sub> fluxes in Figure 10.

*(2) It is unclear why total anaerobic respiration does not change with WTD on p. 12 l. 5. Simulating such changes is one of the key challenges in CH<sub>4</sub> modelling, but is overlooked in this study.*

(2) Response:

In this part of the work, we tested the sensitivity of the simulated CH<sub>4</sub> emissions to input. Anoxic respiration is taken by HIMMELI as input, in mol s<sup>-1</sup> per m<sup>2</sup> of ground surface area, i.e., per the simulated peat column. HIMMELI itself cannot change the total anoxic respiration rate as it is the input, but what it does is that it distributes the given input respiration to the inundated layers of the peat column along the root distribution. Number of those layers depends on WTD and so the anoxic respiration per cubic meter changes with WTD.

As we say above, we agree that simulating anoxic respiration is highly important in CH<sub>4</sub> modelling, however, the case here is that another model (e.g. a soil carbon model of a land surface scheme) has already taken care of it. Most probably the total anoxic respiration rate provided by this other model depends on WTD, but we did not want to set any dependency here, in the mechanistic sensitivity tests, since it would have meant in practice that the test results are valid only when the dependency is as we described it. In this way we keep the tests as more generic and avoid inherent mixing with a soil carbon model.

The idea in our mechanistic tests was to analyze how much and via what pathways the other driving variables (WTD, temperature, LAI) affect the output CH<sub>4</sub> emission rate when the carbon input rate is constant. Given that the anoxic respiration rate largely governs the CH<sub>4</sub> emissions, it is important to standardize it and find out what kind of dependencies there are

inside the CH<sub>4</sub> model alone. As far as we know, this has not been thoroughly analyzed earlier without the mask of changing non-CH<sub>4</sub> carbon processes.

(2) Suggested changes to the manuscript:

We will add text that clarifies this issue on p. 12.

*(3) The fixed fraction of respiration that generates CH<sub>4</sub> (fm in eq. 7) should in theory be fixed at 0.5, rather than be reset to 0.25 for the field study. This fraction directly affects CH<sub>4</sub> generation, but completely overlooks acetotrophic vs hydrogenotrophic methanogenesis.*

(3) Response:

This is one of the parameters that has high uncertainty and indeed affects CH<sub>4</sub> generation directly. It would be great to simulate the different methane production pathways and microbial groups and this way perhaps enable tuning the model to e.g. different peatland types, but we have not done it so far. CH<sub>4</sub> production is only modelled via this one bulk parameter.

Nilsson and Öquist (2009) state in their article that theoretically, the CH<sub>4</sub>/CO<sub>2</sub> quotient from terminal mineralization of soil organic matter in optimal methanogenic conditions ranges from 0 to 0.7, being ~0.5 when carbohydrates are mineralized. Their literature review showed, however, dominance of CO<sub>2</sub>: the observed CO<sub>2</sub>/CH<sub>4</sub> quotient in anoxic incubations had varied from 0.5 to 36,000 with median value in a filtered data set being 6-7. Also models have used ratios other than 50/50, e.g. the CH<sub>4</sub> model by Wania et al. (2010) used CH<sub>4</sub>/CO<sub>2</sub> ratio of 0.1. On this basis, the value 0.25 used in the model calibration is within a realistic range.

We can run the Siikaneva simulations again, with fm of 0.5. However, because the model calibration used 0.25, changing to 0.5 will most probably rise the CH<sub>4</sub> emission level higher than the observations, if we keep the other parameter values, in particular the fraction of NPP allocated to root exudates, the same as now. A compromise that we suggest is to present results from both runs in a supplement, which would also illustrate the effect of changing this parameter.

(3) Suggested changes to the manuscript:

We will discuss this parameter in light of the article by Nilsson & Öquist (2009), in the end of Section 3.2.1. We will rerun the Siikaneva simulation done with the logarithmic layer structure using fm of 0.5, and the result (compared with the original run) will be added as a supplement.

*(4) There was no clear distinction between gaseous and aqueous diffusive fluxes in eqs. 1 – 3, although they are very different above the water table. I presume these are aqueous fluxes below the water table, but what about gaseous transfer above the water table by which gases are exchanged with the atmosphere? Perhaps this can be easily clarified by the authors.*

(4) Response:

Yes, diffusion happens in water below the water table and in the air above it and the model calculates it accordingly. This, including the description of how the flux is calculated at the water-air interface is explained into more detail in Section 3.1.8. "Diffusion in the peat". We are sorry that this is left unclear in the Section 3.1.1 and around the equations 1-3.

(4) Suggested changes to the manuscript:

We will clarify the text in Section 3.1.1 after the equations 1-3 by explicitly mentioning that the diffusive fluxes in the peat are in water below WTD and in air above it.

*(5) The daily time step of the model eliminates the simulation of diurnal variation in temperature, even though this can be an important driver of that in gas exchange.*

(5) Response:

We agree that in this work, which specifically aims at testing the transport model, it would be reasonable to test how the model works if it is run on a shorter time step. The reason for running it on daily time step was that the main plan for HIMMELI is to use it with models that provide daily input and so the present results were needed for that. We can test running the model on a shorter time step.

(5) Suggested changes to the manuscript:

We will test running HIMMELI with realistic input data at frequency shorter than one day, with diurnal variation of soil temperature. Results of this model run will be compared with simulation done on daily timestep, in which input data are daily averages of the previous test. The outcome will be added to Results.

*(6) It is very important to avoid arbitrary parameterizations, such as those associated with the assumed 2 m maximum rooting depth, as these can affect model results in unforeseen ways, and therefore limit the robustness of the model.*

(6) Response:

Maximum rooting depth is, in fact, not fixed to 2 m but it depends on peat depth. If peat depth is less than 2 m, the model uses the peat depth as the maximum rooting depth. In case peat depth is more than 2 m, the model is also prepared to handle the situation, but rooting depth is then set to 2 m according to literature (described in Section 3.1.3). Maximum rooting depth could be changed to a parameter whose value could be determined by the model user but for the current model version, we will not change it.

(6) Suggested changes to the manuscript:

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*(7) The only air-water interface that appears to be modelled is that at the surface of the water table, yet such interfaces exist throughout the soil above the water table. Gas exchange across these interfaces can cause localized anaerobic zones in which CH<sub>4</sub> can be generated.*

(7) Response:

We agree, anaerobic zones can exist above the WTD. However, simulating them would mean increasing the number of uncertain parameters in the model, and simulation of this process would be demanding since, for instance, we do not have corresponding experimental data. As mentioned above, we consider the current approach is robust enough to be used in land surface models.

(7) Suggested changes to the manuscript:

As for the comment (1) above, we will add discussion about how realistic the strict division to oxic/anoxic parts of peat is, on page 7, Section 3.1.2.

*(8) Are different root porosities considered in eq. 19? These are important in plant adaptation to wetlands, as well as in root gas transfer.*

(8) Response:

In the current model version they are not considered. A single porosity is assumed for all the gas-transporting vegetation. They could be implemented in further model versions but similarly

to the previous comment response (7) adding them would mean increasing the number of uncertain parameters in the model.

(8) Suggested changes to the manuscript:

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*(9) CH<sub>4</sub> emissions appear to have limited sensitivity to temperature (p. 15), even though a T response of anaerobic respiration was considered in the model. However field studies indicate a large sensitivity of CH<sub>4</sub> emission to T, as noted later on p. 16, which is likely important in climate warming studies. Has a key process been overlooked here?*

(9) Response:

We regret for having described the test set-up unclearly. In the sensitivity tests described in Sects. 3.2.1 and 4.1, the anoxic respiration was a constant input value that was independent of temperature. This constant respiration was given to HIMMELI that was then driven with different temperatures. Thus, temperature affected the output only by affecting the processes that are included in HIMMELI, that is, inhibition of CH<sub>4</sub> production, aerobic respiration, CH<sub>4</sub> oxidation, and the transport processes. Therefore, the result of the test tells about the sensitivity of these other processes to temperature.

When running HIMMELI for the Siikaneva site, we used non-constant simulated anoxic respiration, part of which was produced using the temperature dependent Q10 model. In this case both anoxic respiration and output CH<sub>4</sub> emission correlated with temperature, however, this was at least principally due to the input correlating with temperature, which is always the case when HIMMELI is used together with an independent carbon cycle model.

According to literature (e.g. Nilsson & Öquist, 2009), CH<sub>4</sub> production is more sensitive to temperature than CO<sub>2</sub> production, or conversely, the CO<sub>2</sub>/CH<sub>4</sub> quotient decreases when temperature increases. In a way this has now been taken into account to some extent since increasing temperature reduces O<sub>2</sub> solubility and thus the dissolved O<sub>2</sub> concentration available for inhibiting CH<sub>4</sub> production and enhancing CH<sub>4</sub> oxidation is reduced.

(9) Suggested changes to the manuscript:

We will clarify the role of the input respiration in different tests, in the section about the tests (3.2) and in the Results and discussion section. We will add a figure that shows the correlation of soil temperature with anoxic respiration used as input in the Siikaneva simulations, as well as correlation between temperature and modelled CH<sub>4</sub> emissions.

*(10) Is it realistic that CH<sub>4</sub> emissions should increase with WTD (p. 15), or is root-mediated O<sub>2</sub> transport overestimated? Is root growth constrained by O<sub>2</sub> below the WT? Or is this model result an artefact of assumptions regarding WTD and anaerobic respiration noted in (2) above?*

(10) Response:

The simple answer to this question is that we do not know how realistic the root oxygen transport is. Here we indeed again face the fact that in our tests, input respiration was not dependent on WTD. In reality, and with a model that simulates anoxic respiration dependent on WTD, probably the anoxic respiration rate per peatland surface area would decrease with decreasing WTD and therefore also the CH<sub>4</sub> emissions would decrease, despite of the decreasing root transport of O<sub>2</sub> into the inundated soil. But now when WTD had no impact on the anoxic respiration rate, the result was reverse, which is an interesting result as such and not discussed earlier since non-CH<sub>4</sub> carbon processes are masking the dynamics of CH<sub>4</sub> processes

There are a few previous CH<sub>4</sub> models that also simulate the O<sub>2</sub> transport to the peat and the consequent O<sub>2</sub> concentrations affect different processes in the soil (e.g. Wania et al., 2010, Riley et al., 2011). However, since the observational data on O<sub>2</sub> transport is scarce or nonexistent, it is by definition not possible to validate these results. Our analysis shows that it should be done.

Root mass is vertically distributed according to the exponential function (Eq. 4). This means that the root transport capacity is small in the bottom peat layers.

(10) Suggested changes to the manuscript:

We will write a more thorough explanation of how anoxic respiration depended on WTD in the first paragraph of Section 4.1, 'Model sensitivity to input data'.

*(11) In the Xu et al. (2016) paper cited in the manuscript, 40 existing CH<sub>4</sub> models were reviewed. In many of these models, the issues raised above are explicitly addressed, but some key challenges to further development of these models were raised. The question to be addressed when considering this manuscript for publication is does the model proposed here build upon this earlier work by providing further insight into the key processes by which CH<sub>4</sub> emissions are controlled and thereby addressing these challenges? Or is this just another empirical model of CH<sub>4</sub> emissions, the parameterization of which is site- and model-specific without reference to earlier modelling work, and therefore of limited interest to the larger modelling community. Unless the authors can provide convincing responses to the points raised above, then I fear the latter.*

(11) Response:

We acknowledge the fact that HIMMELI does not bring any new processes as such into the CH<sub>4</sub> model world and the process descriptions largely are from earlier models, which we explicitly mention on p3, lines 11-12. HIMMELI was developed in order to have a CH<sub>4</sub> module that could be plugged into different peatland carbon models and that simulates transport of all CH<sub>4</sub>, O<sub>2</sub> and CO<sub>2</sub>. The parameterization in the current manuscript is based on only one peatland site, however, the aim has been to have physically sound parameter values. When moving to other peatlands and especially if using HIMMELI in large-scale methane modeling, the model needs to be re-calibrated.

We agree that we explained very vaguely how HIMMELI relates to the existing methane models. Xu et al. (2016) listed 40 terrestrial ecosystem models for CH<sub>4</sub> cycling. However, when considering only their CH<sub>4</sub> emission parts, this number seems to be slightly reduced. For instance, Ringeval et al. (2011) say that they included the Walter et al. CH<sub>4</sub> model in ORCHIDEE and Spahni et al. (2011) that they applied LPJ-WhyMe in LPI-Bern for biogeochemical modelling of CH<sub>4</sub> emissions.

Although HIMMELI does not include all processes that already exist in some models (e.g. alternative e<sup>-</sup> acceptors, anaerobic CH<sub>4</sub> oxidation), it is among the most complete models considering the transport of compounds. According to Xu et al., there are only 5 models that simulate all vertically resolved biogeochemistry, O<sub>2</sub> availability to CH<sub>4</sub> oxidation, and three pathways of CH<sub>4</sub> transport. Of these, the Xu model (Xu et al. 2007), CLM-Microbe (Xu et al. 2014) and VISIT (Ito & Inatomi, 2012) do not explicitly simulate O<sub>2</sub> transport between the atmosphere and peat. On the other hand, LPJ-WhyMe (Wania et al. 2010), a revised multi-substance version of TEM (Tang et al. 2010) and a recent model by Kaiser et al. (2017) - that were not included in the list by Xu et al. -- do simulate all these. HIMMELI also simulates CO<sub>2</sub> transport via all three transport pathways. This is not a common feature in CH<sub>4</sub> models: to our knowledge, only the multi-substance version of TEM (Tang et al. 2010) and the Segers model (Segers & Leffelaar, 2001) included it.

Xu et al. (2016) raised some needs and key challenges to further development of the CH<sub>4</sub> models. Some of them are not relevant for HIMMELI as they concern complete peatland ecosystem models -- however, we admit that HIMMELI does not address all of those that were relevant. We can, however, point out two issues. Firstly, Xu et al. emphasized that the models should consider the vertical distribution of processes, which is something that HIMMELI does. Secondly, Xu et al. stated that well-validated CH<sub>4</sub> modules should be included in Earth system modeling frameworks. Although not mentioned in the manuscript, the main goal of HIMMELI is to use it as a module in large-scale land surface models (JSBACH, JULES) that are part of ESMs.

When it comes to the modeling community's interest in the manuscript, we think that especially because this model does include components similar to earlier CH<sub>4</sub> models, the results of the sensitivity analysis should be interesting. Xu et al. (2016) wrote: "Furthermore, evidence demonstrating that incorporating all of these processes would lead to more accurate prediction is needed". We think our paper is a statement in this type of discussion since it indicates that A) although vertically resolved transport and oxidation processes have significance, the CH<sub>4</sub> emissions simulated by this type of models are largely determined by the CH<sub>4</sub> production rate and B) adding complexity like e.g. transport of oxygen and effect of O<sub>2</sub> concentration on the process rates can have a high impact on the output. However, because of general lack of data, it remains unclear if anyone has validated the realism of the oxygen processes.

(11) Suggested changes to the manuscript:

In the Introduction, we will clarify the aim of HIMMELI and describe how this model relates to earlier methane models by adding the above text that refers to the review by Xu et al. (2016).

## REFERENCES

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