

Dear Editor and Referees,

We have now revised the manuscript. We followed the suggestions and comments of the Referees and tried to clarify the message in places that were unclear. In addition, thanks to the good comments, we noticed that a couple of additional major changes were necessary. We hope that our response is satisfactory and the manuscript is now suitable for publication.

Below please find: A) a list of the relevant changes we have made to the manuscript, B) the original response letters to the Referees, in which we have added **in blue text** the changes we really made in the manuscript, and C) the marked-up version of the manuscript. However, the page and line numbers refer to the manuscript version (the separate pdf) in which **no markup** is shown.

A) The relevant changes we made to the manuscript

1. As Referee #1 suggested to add CO₂ fluxes in Fig. 10 (now Fig. 13), we also compared the simulated CO₂ with respiration rates observed at Siikaneva. We noticed that the CO₂ emissions simulated with the previous parameterization were too high, especially due to aerobic respiration rates. Therefore, we decided to change the parameter values. The parameter controlling aerobic respiration is now based on the observed respiration at Siikaneva, and other parameter values are also taken from general literature. The new parameterization is described in the new Section 3.2 and it also affected the description of simulating anoxic respiration in App. B, p. 26 l. 13-20. This change improved the CO₂ emission levels. Otherwise the test results are very similar to the earlier version, there were no essential changes. The exact values (in tables and the Results and discussion section) just have changed slightly, and naturally all results in the figures were re-plotted (figures other than Fig. 1). The CO₂ fluxes are discussed on p. 23 l. 6-11.
2. The Reviewers asked about the effect of eliminating diurnal temperature variation with daily time step. We tested this and thanks to the test, noticed that although steady-state temperature does not have any significant effect on the output fluxes, *change* in peat temperature did affect, by affecting gas solubilities. Therefore, we added a temperature transition test. The main changes related to the temperature transition are in p. 14 l. 9 & 14-16; p. 19 l. 18-23, and Fig. 8. This also helped us to understand why the model predicted CH₄ emission peaks at Siikaneva in 2010, see new text on p. 23, l. 13-24.
3. We realized that it was not reasonable to have 0°C temperature in the steady-state temperature test as this model version does not yet take into account freezing of water. So we removed those results from the analysis (Table 2 and Fig. 7, previously Fig. 6) and mention this limitation now in model description, p. 6 l. 20-21.
4. We added a model vs. observations comparison on another peatland site Lompolojänkämä. The main changes are in Sects. 3.3.4 'Comparison of HIMMELI...', 3.4 'Peatland sites and data' (we re-organized the text by adding a separate section on input data preparation), and 4.4 'Comparison of modelled and measured CH₄ fluxes'. Figure 14 b. shows the Lompolojänkämä results. Also a new author, responsible for the new site data, was added.
5. We added text in Introduction p. 3, l. 7-27. It clarifies the aim of HIMMELI and describes how this model relates to earlier methane models. Also the aims of the paper were partly re-formulated, p. 4, l. 5-9.
6. P. 7 l. 11-15: new text about the time step. The new test on shorter time step is in Sects. 3.3.2 and 4.2. and new figures 2. and 12., related to this test, were inserted.
7. P. 7, l. 26-29: we explain why the strict division of air- and water-filled peat is justified.
8. P. 9, l. 13-16: we added text about alternative electron acceptors.
9. P. 11 l. 1-8: we added text about bubble movement.
10. P. 12, Eq. 19: we noticed an error in the equation and removed area *A* from the denominator.
11. We re-formulated Section 3.3 'Model testing' because the new tests were added and because we wanted to clarify the aim of testing the model on the peatland sites.
12. P. 14, l. 20-27: we added clarifying text about why and how the anoxic respiration was independent of WTD and temperature.

13. P. 18, first chapter: we added text that still clarifies the role of anoxic respiration in these tests.
14. P. 22, l. 16-22: we added comparison of our input anoxic respiration to literature values, to show that the magnitude of the input respiration was realistic.
15. The last figure was divided into two, Figs. 14 and 15. Fig. 14 now compares modelled and measured CH₄ fluxes at two peatland sites and Fig. 15 shows old and new correlation plots.

B) Responses to the Referees

Referee comments are typed in *italics*. They are followed by our earlier responses as black plain text and the changes we really made as blue text. [The blue page and line numbers refer to the manuscript version in which no markup is shown.](#)

Referee #1

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 CH₄ production, as noted in p. 14 and Fig. 11. Anaerobic respiration therefore needs to be explicitly simulated as part of any CH₄ model, rather than optimized for site conditions as done here, as it directly determines modelled CH₄ 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 CO₂ fluxes with modelled CH₄ 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 CH₄ emissions. However, the target of our work was to produce a module that simulates only the transport and oxidation of CH₄. The reason for this is that there are soil carbon models that simulate anoxic respiration and the interface to a CH₄ 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 CH₄ 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 CH₄ 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 CH₄ 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 CO₂ fluxes into Fig. 10 is indeed a good suggestion.

(1) Suggested changes to the manuscript [and the changes we made](#):

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 added text on p. 3 l. 7-10.](#)

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.

[Role of Siikaneva has been clarified especially in Sect. 3.3.4.](#)

[Comparison with Lompolojännkä is reported mainly in Sects. 3.4., 4.4 and Appendix B. Fluxes are plotted in Fig. 14.](#)

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

[This was added, p. 7, l. 26-29.](#)

We will add CO₂ fluxes in Figure 10.

[These fluxes were added, now Fig. number 13.](#)

(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 CH₄ modelling, but is overlooked in this study.

(2) Response:

In this part of the work, we tested the sensitivity of the simulated CH₄ emissions to input. Anoxic respiration is taken by HIMMELI as input, in mol s⁻¹ per m² 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 CH₄ 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 CH₄ emission rate when the carbon input rate is constant. Given that the anoxic respiration rate largely governs the CH₄ emissions, it is important to standardize it and find out what kind of dependencies there are inside the CH₄ model alone. As far as we know, this has not been thoroughly analyzed earlier without the mask of changing non-CH₄ carbon processes.

(2) Suggested changes to the manuscript:

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

[This was added, now page 14, l. 21-27.](#)

(3) The fixed fraction of respiration that generates CH₄ (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 CH₄ generation, but completely overlooks acetotrophic vs hydrogenotrophic methanogenesis.

(3) Response:

This is one of the parameters that has high uncertainty and indeed affects CH₄ 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. CH₄ production is only modelled via this one bulk parameter.

Nilsson and Öquist (2009) state in their article that theoretically, the CH₄/CO₂ 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 CO₂: the observed CO₂/CH₄ 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 CH₄ model by Wania et al. (2010) used CH₄/CO₂ 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 CH₄ 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.

[What we did, in the end, was to run all the tests using *fm* of 0.5. We also discuss this parameter on p. 13, l. 9-14.](#)

(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.

[This was done, p. 7 l. 6.](#)

(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.

[We did this test. It is described in Sections 3.3.2 and 4.2.](#)

(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 CH₄ 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.

[This was added, p. 7, l. 26-29.](#)

(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) CH₄ 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 CH₄ 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 CH₄ production, aerobic respiration, CH₄ 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 CH₄ 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), CH₄ production is more sensitive to temperature than CO₂ production, or conversely, the CO₂/CH₄ quotient decreases when temperature increases. In a way this has now been taken into account to some extent since increasing temperature reduces O₂ solubility and thus the dissolved O₂ concentration available for inhibiting CH₄ production and enhancing CH₄ 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 CH₄ emissions.

New text has been added on p. 14, l. 22-27 and p. 18 l. 9-11. Fig. 15 shows the temperature correlations in the Siikaneva test.

(10) Is it realistic that CH₄ emissions should increase with WTD (p. 15), or is root-mediated O₂ transport overestimated? Is root growth constrained by O₂ 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 CH₄ emissions would decrease, despite of the decreasing root transport of O₂ 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-CH₄ carbon processes are masking the dynamics of CH₄ processes

There are a few previous CH₄ models that also simulate the O₂ transport to the peat and the consequent O₂ concentrations affect different processes in the soil (e.g. Wania et al., 2010, Riley et al., 2011). However, since the observational data on O₂ 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'.

The new text on p. 14, l. 22-29 explains this, and we also added a short clarifying sentence on p. 18. l. 7-9.

(11) In the Xu et al. (2016) paper cited in the manuscript, 40 existing CH₄ 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 CH₄ emissions are controlled and thereby addressing these challenges? Or is this just another empirical model of CH₄ 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 CH₄ 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 CH₄ module that could be plugged into different peatland carbon models and that simulates transport of all CH₄, O₂ and CO₂. 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 CH₄ cycling. However, when considering only their CH₄ emission parts, this number seems to be slightly reduced. For instance, Ringeval et al. (2011) say that they included the Walter et al. CH₄ model in ORCHIDEE and Spahni et al. (2011) that they applied LPJ-WhyMe in LPI-Bern for biogeochemical modelling of CH₄ emissions.

Although HIMMELI does not include all processes that already exist in some models (e.g. alternative e⁻ acceptors, anaerobic CH₄ 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, O₂ availability to CH₄ oxidation, and three pathways of CH₄ 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 O₂ 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 CO₂ transport via all three transport pathways. This is not a common feature in CH₄ 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 CH₄ 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 CH₄ 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 CH₄ 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 CH₄ emissions simulated by this type of models are largely determined by the CH₄ production rate and B) adding complexity like e.g. transport of oxygen and effect of O₂ 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).

[We added a shortened version of the text and some clarification in Introduction, p. 3, l. 15-26 and p. 4 l.1-2.](#)

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Referee #2

1) *This manuscript presents a sensitivity analysis of a methane module that could be included in peatland models. The authors argue that the novelty of this study is that the model has been developed independent of a full peatland carbon model and can then be tested for sensitivity allowing for dependencies within the methane models itself to be assessed separately from the entire C model. The fact that it is a module without the complete C cycling that feeds input to the methane module, makes it difficult to assess the ability of the model to estimate fluxes as the test that compares it to field-measured fluxes did not optimize the anoxic respiration input and this would actually be generated from the entire peatland C model. Also, sensitivities are difficult to assess this way as important drivers (e.g., temperature driving CH₄ production) are not included as this would happen in the other part of the peatland C model that would drive anoxic respiration rates.*

(1) Response:

We agree with the Referee that it is difficult to evaluate the model's ability to predict CH₄ fluxes and sensitivities to input when it does not include the whole carbon cycle. The reason for developing this kind of methane model was to produce a module that can be used in different purposes, as a platform for specific studies on methane processes, but principally as a component of large-scale biosphere models that provide the anoxic respiration input. We believe it can be useful for the community. For instance, the CH₄ model of Walter & Heimann (1996) has been utilized in several peatland ecosystem modelling frameworks to simulate methane (e.g. in Ringeval et al. 2011, van Huissteden et al. 2009).

We considered the test with Siikaneva data (Sections 3.2.3, 4.2 and 4.3) as a test of whether HIMMELI produces realistic output, as we aimed at using as realistic input respiration as possible in this test. On the other hand, as written in the manuscript, we especially think that as the anoxic respiration rate largely governs the CH₄ emissions, it is important to standardize it and find out what kind of dependencies there are inside the CH₄ model alone, given that it usually takes a relatively large portion of a complete peatland carbon model.

(1) Suggested changes to the manuscript [and the changes we made](#):

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

[We added text in Introduction, p. 3 on lines 7-10.](#)

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 parameterisation fits to other peatland sites.

[We re-formulated Section 3.3.4, in order to clarify the role of the tests on Siikaneva and the other site Lompolojännkä. The Lompolojännkä site is described in Sect. 3.4.2.](#)

(2) *Aside from testing the sensitivity of a methane model outside of a full C model, the novelty of the model itself is not clear. The way in which methane production, oxidation and transport is considered in the model appears to be largely developed according to methods used in previous models and therefore it is not clear what improvement is expected here. The way in which ebullition is handled, for example, is quite simplistic and not consistent with literature that clearly illustrates trapping of free-phase gas over time as opposed to release as soon as a bubble is formed (e.g., Comas et al., 2014; Ramirez et al., 2015). I think a clear justification of why another peatland CH₄ model is needed must be included to illustrate the utility of this model.*

(2) Response:

About ebullition: please see our responses to your comments number (11) and (14).

We acknowledge the fact that HIMMELI does not bring any new processes into CH₄ modelling and the process descriptions are based on earlier models. This is mentioned on P3, lines 11-12. We wanted to produce a model that simulates the transport of all CH₄, O₂ and CO₂ that is not a common feature among CH₄ models. We decided that rather than taking directly one of the existing model codes that are developed with and thus closely connected to some

biosphere model, we would systematically start from fundamental elements and combine the process descriptions in a format that can be flexibly applied for different uses as, for instance, the peat column structure is not fixed.

Although HIMMELI does not include all processes that already exist in some models (e.g. alternative e^- acceptors, anaerobic CH_4 oxidation), it is among the most complete models considering the transport of compounds. According to Xu et al. (2016), who reviewed 40 existing terrestrial ecosystem models for CH_4 cycling, there are only 5 models that simulate all these: vertically resolved biogeochemistry, O_2 availability to CH_4 oxidation, and three pathways of CH_4 transport. Of these 5, the Xu model (Xu et al. 2007), CLM-Microbe (Xu et al. 2014) and VISIT (Ito & Inatomi, 2012) do not explicitly simulate O_2 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_2 transport via all three transport pathways. To our knowledge, only the multi-substance version of TEM (Tang et al. 2010) and the Segers model (Segers and Leffelaar, 2001) included it.

We think that as the anoxic respiration rate largely governs the CH_4 emissions, it is important to standardize it and find out what kind of dependencies there are inside the CH_4 model alone, given that it takes a relatively large portion of a complete peatland carbon model. Here the fact that HIMMELI contains similar components as other methane transport models means that the results reveal and clarify inherent assumptions and process dynamics in the other models.

(2) Suggested changes to the manuscript:

We will justify the necessity of the new model by adding the contents of the above text (reference to Xu et al. 2016) in the Introduction.

[We added text in Introduction, p. 3 on lines 15-27.](#)

(3) Page 2, Line 5: Maybe the 2nd largest anthropogenic radiative forcing after CO_2 ? Water vapour causes the greatest radiative forcing in the atmosphere, followed by CO_2 and then CH_4

(3) Response:

Agreed.

(3) Suggested changes to the manuscript:

We will correct this sentence: "...inducing the second largest radiative forcing among well-mixed greenhouse gases."

[This was done, p. 2 l. 6.](#)

(4) Page 2, Line 13: Saying no other alternative electron acceptors exist is a bit extreme. Many freshwater wetlands will have cycling of NO_3 , Fe, SO_4 , etc., in addition to CH_4 production. I suggest rewording this sentence.

(4) Response:

Yes, we agree.

(4) Suggested changes to the manuscript:

We will remove this sentence.

[We removed it \(p. 2 l. 14\).](#)

(5) Page 4, Line 28: I guess 45-60% is meant (as opposed to : : :). This happens throughout the manuscript in my version.

(5) Response:

The manuscript preparation guidelines of this journal say: "A range of numbers should be specified as "a to b" or "a...b". The expression "a-b" is only acceptable in cases when no confusion with "a minus b" is possible." We thought it would be clearest to use the same convention consistently throughout the manuscript and therefore the expression "a...b" everywhere but we can change this.

(5) Suggested changes to the manuscript:

We leave the "a...b" expression only in tables but within the text change it to "a to b".

[This was done.](#)

(6) Page 5, Lines 1-3: And also, peat properties and pore sizes are likely to vary within and between peatlands based on composition of the peat (i.e., sedge vs. wood vs. moss) as well as decomposition status.

(6) Response:

Yes, true, that is relevant information here. Thank you for pointing out these.

(6) Suggested changes to the manuscript:

We will add this information on Page 5.

[We added this on p. 5 l. 21-22.](#)

(7) Page 5, line 7: the effect of tortuosity on the diffusion coefficient indicates that it is not only the porosity that is important, but the interconnectivity and shape of that porosity and probably the pore size distribution

(7) Response:

Yes, this is a good point. We are sorry for the inadequate piece of text.

(7) Suggested changes to the manuscript:

We will modify this text so that it also describes the significance of tortuosity.

[We changed this, p. 5 l. 25-27.](#)

(8) Page 6, Line 7: In reality WT is the not the divide between water-filled and partially water-filled pore space. Above the WT there is always some fully saturated layer as the capillary fringe. In practice in the model it doesn't make a difference as the boundary would instead be the capillary fringe, but the way it is written here is technically incorrect.

(8) Response:

We agree, this is an incorrect statement as it is, this should refer only to the model.

(8) Suggested changes to the manuscript:

We will correct this sentence to: "In the model, WTD is taken as a strict divider of the peat into water-filled and air-filled parts."

[This was done, p. 7 l. 21.](#)

(9) Page 6, Line 11: When WT is above the surface it can become oxygenated by windmixing. Is this considered?

(9) Response:

Yes, windmixing can affect the O_2 concentrations but this is not considered in the model yet. The model naturally is a rough simplification of reality: so far it assumes a pure water layer on top of the peat surface, although there often is vegetation growing in the peat. Vegetation would hinder the windmixing via affecting wind speed and generally modifying the physical conditions affecting thin boundary layers regulating gas transfer across the water-air interface. These processes are not fully understood even for open water surfaces of inland water bodies (we are also working with these issues) and in our opinion the inclusion of partly unknown processes is out of the scope of the present manuscript.

(9) Suggested changes to the manuscript:

We will discuss this point in the Section 3.1.2 in which the possible water layer on top of the peat surface is mentioned.

[Discussion was added, p. 8 l. 2-3.](#)

(10) Equation 7: What about inhibition by other electron acceptors? I know you are not following them in the model, but they could be important in some fen systems. Is CH_4 production from the peat matrix accounted for – anaerobic respiration is driven by rooting depth, but CH_4 could be produced from other substrates.

(10) Response:

We think that other electron acceptors are an important issue. We did not include them in the model because we thought their concentrations depend on site characteristics, such as the water source, and it would be difficult to estimate them. Therefore, these estimates would necessarily not improve the accuracy of the model. However, given that our results (and also earlier works) indicate that methane production rate largely drives the simulated emissions and the oxygen

inhibition thus plays a significant role, including other e- acceptors could possibly be a way to take into account site differences, for instance, bog vs. fen. This could be done in future model versions.

In the current model version, anoxic respiration is one bulk input stream and HIMMELI does not take a stand on what organic compounds are decomposed, whether they are root exudates or other substrates. For simplicity, everything is distributed with the root mass except in the case that peat depth exceeds 2 m when some respiration also is allocated in the rootless peat layers. This choice (as opposed to distributing the input e.g. evenly across the peat column) was motivated by the fact that recently fixed carbon seems to be the main source of methane. For instance, according to Oikawa et al. (2017), less than 5% of CO₂ and CH₄ emissions originate from soils below 50 cm in flooded peatlands. However, in case that HIMMELI is used in a context where it is essential to simulate the different carbon sources, it is not a big task to modify the code so that this becomes possible.

(10) Suggested changes to the manuscript:

We will add text/discussion about the possible other electron acceptors and distribution of input carbon in the Section 3.1.3 on CH₄ production.

Discussion was added, p. 9 I. 2-6 and 13-16.

(11) Equation 11: Is this really realistic? This would allow a bubble to form, but that doesn't mean that ebullition occurs. Also, once bubbles form, they are often trapped and this affects the concentration gradients and also the ebullition fluxes. A very large bubble release is likely to provide such a high concentration when released that even if the WT is below the surface, not all the CH₄ will be oxidized (see page 14, line 15 in the manuscript).

(11) Response:

We agree with the Referee that after a bubble has been formed there are still several processes that take place before the bubble reaches the surface and contributes to the CH₄ flux to the atmosphere. For instance, the bubbles still need to traverse through the peat column up to the atmosphere. Also, like the Referee mentions, during the time that the bubbles travel upwards towards the atmosphere they constantly interact with the surrounding pore water and hence alter e.g. the CH₄ concentration gradients.

Such processes are still missing from most of the peatland CH₄ models (Xu et al., 2016), including HIMMELI. This is most likely because relatively little is known about bubble movement in peat and how to describe it accurately in models, although there are some attempts to model this process (Ramirez et al., 2015). In general, bubble movement in porous media is a highly complex problem, which depends on the fine-scale structure of the media in which the bubbles are moving in. How to incorporate such complex phenomenon in a simple, yet accurate way in peatland CH₄ cycling models is still unsolved. However, as it happens, we are at the moment preparing a manuscript in which we are comparing different ebullition modelling approaches and one of them incorporated a simple scheme to take into account the bubble movement. Nevertheless, as mentioned this is a topic for the other study.

Considering the reviewer's comment about the page 14, line 15: in this manuscript direct ebullition to the surface takes place only when WTD is above the surface. If WTD is below surface, then the CH₄ in the bubbles is released to the lowest air layer from where it is transported via diffusion in the air-peat column to the atmosphere. Hence even large bubbles are first released to the bottom air layer below the peat surface, before reaching the atmosphere. We argue that this is how it happens also in reality and hence is the correct way to describe this process in a model.

(11) Suggested changes to the manuscript

We will discuss the points mentioned above (how the bubble movement would happen in reality, compared with the model) in Section 3.1.7. In addition, we will clarify the sentence on page 14. It now is: "...the direct ebullition fluxes to the atmosphere were zero when WTD was below the peat surface" but we will rephrase it: "ebullition to the atmosphere occurred only when WTD was at or above the peat surface". We hope this slightly modified version is clearer.

Discussion was added, p. 11 I. 1-8 and the sentence was clarified.

(12) Page 12, Lines 20-25: Was the model parameterized with the data from Siikaneva? If so, how appropriate was the test?

(12) Response:

Yes, the parameter set used in this study was a combination of literature values and values set by calibrating HIMMELI with Siikaneva data. In this sense the test was not appropriate for evaluating the model fit. However, the purpose of this test was to demonstrate that combined with realistic input, HIMMELI does output realistic CH₄ fluxes, which is not so evident if looking only at the mechanistic sensitivity tests. We admit this is not said very clearly in the manuscript. In addition, we think that comparing the explanatory power of input respiration only with the input + HIMMELI combination is continuation to the sensitivity tests, as it addresses the question of how necessary the transport+oxidation model is.

(12) Suggested changes to the manuscript:

As already mentioned (point 1), 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 parameterisation fits to other peatland sites.

[We changed the parameterization of the model so that it is not anymore optimized for Siikaneva \(Sect. 3.2\) and the model is tested also with data from another site Lompolojänkää \(main additions in Sects. 3.4., 4.4 and Appendix B\).](#)

(13) Page 16, lines 26-27: Does this illustrate that evaluating sensitivities in the methane only module, especially when production rates are not appropriately driven by changing conditions, is problematic? Temperature is a very important driving factor for CH₄ production, but it is not included in the way the module is constructed making it very difficult to interpret the actual sensitivities of the model.

(13) Response:

We do not think it is problematic. The purpose of the mechanical sensitivity tests was precisely to find out what kind of physical mechanisms govern the behavior of this CH₄-only-module, which facilitates its evaluation. For instance, we find it relevant knowledge that the impact of temperature on the processes included in HIMMELI is principally mediated via gas solubilities by affecting the concentrations of dissolved O₂.

Perhaps we misunderstand the Referee's comment but temperature is included in the way that the module is constructed. We agree that simulating anoxic respiration is highly important in CH₄ modelling, however, the idea here is that another model (e.g. the 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 temperature, but we did not want to set any dependency here since it would have meant, in practice, that the test results are valid only when the dependency is as we described it.

(13) Suggested changes to the manuscript:

We will emphasize on p. 16 that finding different temperature sensitivities when the carbon input is independent of temperature is not a downside but new relevant information for CH₄ model development.

[A sentence was added, p. 21 l. 12-13.](#)

(14) Page 17, line 10: In this model, the peat column and layering is not important, but what about if the gas is being trapped prior to ebullition or even once mobilized from one layer and then trapped in another (e.g. Comas et al., 2015). We know this happens in reality, but it is not included in this model. If it was how would the results of the study change?

(14) Response:

Like the Reviewer mentions, bubble movement in peat is not included in HIMMELI. However, as mentioned before, we are preparing a manuscript about comparing different ebullition modelling approaches and one of the approaches that are compared in that study included a simple bubble movement scheme. We will shortly describe our findings in that study now here. As expected, if bubble movement (attach, detach) are included, then smaller amount of bubbles reach the surface, i.e. ebullition flux to the atmosphere is smaller. On the other hand, the bubbles that are attached during their ascent release CH₄ to the pore water if the pore water CH₄ concentration is low enough (Henry's law). Hence, the vertical CH₄ concentration gradient is smoother when compared to the case without bubble movement. However, we did not test

different layerings with the other ebullition modelling approaches and thus, unfortunately, cannot say whether the model would be more sensitive to the layering if the ebullition model took trapping of gas into account.

(14) Suggested changes to the manuscript:

None, except what was suggested for the comment 11.

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Referee #3

The Global Methane cycle is currently a topic of much interest following the near-zero growth in atmospheric methane concentrations in the early 2000's and its renewed growth since 2007. Various papers have suggested specific sources, including emissions from wetlands, and more recently changes in the atmospheric CH₄ sinks, as possible explanations. Wetlands globally are the largest single source of methane, anthropogenic or natural. Boreal wetlands are significant and could become more important still with the faster warming of the Arctic and high northern latitudes. The Wetland Model Intercomparison (cited paper by Melton et al., 2013) highlighted the current performance of wetland models and the large range of wetland areas and methane fluxes simulated by the participating models. The recent paper by Saunois et al. (2016) on the Global Methane Budget removed some of this model uncertainty by prescribing the wetland extent/area.

(1) I was expecting the present paper to make this connection to the bigger picture. From the material presented, it is very unclear what the intended application of this new model is (local, regional, global??), how it would be used in practice (standalone or coupled) and indeed what advantage it offers over those mentioned in the paper (i.e., Peatland-VU, CLM) and those already in the literature (see cited paper by Xu et al.).

(1) Response:

We are sorry that we failed to describe the aim of this model clearly. The motivation for our work was to produce a methane model that can be used in different purposes, ranging from a component of a large-scale biosphere model to a platform for specific studies on methane processes. Therefore it is not clearly stated how the model should be used; the idea is that it can be used within different environments and scales. What is true is that most probably the parameter

values we used are not always optimal but the model needs to be re-calibrated, especially if using it in large-scale modelling. This we do not mention in the manuscript, but it should be done.

We acknowledge the fact that HIMMELI does not bring any new processes into CH₄ modelling and the process descriptions are based on earlier models. HIMMELI was developed in order to have a CH₄ module that could be plugged into different peatland carbon models and that simulates transport of CH₄, O₂ and CO₂. Rather than taking, modifying and testing directly one of the existing model codes that are developed e.g. with some biosphere model, we decided to systematically start from fundamental elements and combine the process descriptions in a format that can be flexibly applied for different uses as, for instance, the peat column structure is not fixed. We believe this is the advantage: HIMMELI is intended to be a CH₄ module that can be used with different input sources. On the other hand, we think that as the model has components similar to other methane models, results of the sensitivity analysis can be generally relevant. In many models, oxygen is simulated but is it known whether the fluxes and effects are realistic.

We also agree that we explained very vaguely how HIMMELI relates to the existing methane models. Xu et al. (2016) listed 40 terrestrial ecosystem models for CH₄ cycling. However, when considering only their CH₄ emission parts, this number seems to be slightly reduced. For instance, Ringeval et al. (2011) wrote that they included the Walter et al. CH₄ model in ORCHIDEE and Spahni et al. (2011) that they applied LPJ-WhyMe in LPI-Bern for biogeochemical modelling of CH₄ emissions.

Although HIMMELI does not include all processes that already exist in some models (e.g. alternative e⁻ acceptors, anaerobic CH₄ 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, O₂ availability to CH₄ oxidation, and three pathways of CH₄ 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 O₂ 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 CO₂ transport via all three transport pathways. This is not a common feature in CH₄ models: to our knowledge, only the multi-substance version of TEM (Tang et al. 2010) and the Segers model (Segers and Leffelaar, 2001) included it.

(1) Suggested changes to the manuscript [and the changes we made](#):

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

[This was added in Introduction, p. 3, l. 7-27.](#)

(2) The model considers the major CH₄ release pathways to the atmosphere (diffusion, plant vascular transport and ebullition) and includes oxidation by O₂. O₂ is the only electron acceptor considered. What about others?

(2) Response:

We agree that other electron acceptors are an important issue. We did not include them in the model because we thought their concentrations depend on site characteristics, such as the water source, and it would be difficult to estimate them. Therefore, these estimates would not necessarily improve the accuracy of the model. However, given that our results (and also earlier works) indicate that methane production rate largely drives the simulated emissions and the oxygen inhibition thus plays a significant role, including other e⁻ acceptors could possibly be a way to take into account site differences, for instance, bog vs. fen. This could be done in model version 2.

(2) Suggested changes to the manuscript:

We will add text/discussion about the possible other electron acceptors and distribution of input carbon in the Section 3.1.3 on CH₄ production.

[Discussion was added, p. 9 l. 13-16 \(and 2-6 about carbon distribution\).](#)

(3) I am little concerned at the realism of completely oxic layers sitting above the watersaturated anoxic layers. In reality, one might expect a continuous transition, as acknowledged by the authors.

(3) Response:

We 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 CH₄ transport and oxidation', water-filled, anoxic sites can occur above it. In our opinion, however, it is uncertain to what extent the model-based estimate of CH₄ emissions of a peatland site or larger area would be improved e.g., by assuming a certain volume of anoxic microsites in the peat above the WTD. 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. In addition, simulating partially anoxic peat layers would bring new uncertain parameters in the model. On these grounds, we think this strict division to anoxic and oxic parts is a robust and simple approach.

(3) Suggested changes to the manuscript:

We will add discussion about how realistic is the strict division to oxic/anoxic parts of peat, on page 7, Section 3.1.2. [This was added, p. 7, l. 26-29.](#)

(4) The model runs on a daily timestep. This may be appropriate for large-scale decadal or centennial runs but no justification is given. How was this timestep selected and what are the implications for the modelled methane fluxes?

(4) Response:

The reason for running the model on a daily time step was that the main plan for HIMMELI is to use it with models that provide daily input and so these test results are useful for that purpose. However, we agree that in this work that specifically aims at testing the transport model it would be reasonable to test the effect of time step length on e.g. daily CH₄ fluxes. So far we have not done it and thus do not know the effect on output CH₄ fluxes, but we can test this.

(4) 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 (as Referee 1 asked about diurnal temperature variation). Results of this model run will be compared with simulation done on daily time step, in which input data are daily averages of the previous test. The outcome will be added to results.

[We did this test. It is described in Sections 3.3.2 and 4.2.](#)

(5) Many of the model parameters are optimised using the measurements made at a site in southern Finland (see Table 1, p. 30). These results are included in a second paper (Susiluoto et al., 2017), which is in preparation. This makes it hard to assess their significance, especially in the light of the statement The uncertainty of some of these parameters is rather high, and a more complete analysis can be found in Susiluoto et al. (2017, in prep.).

(5) Response:

This is true. Originally we planned to include a detailed description of the MCMC parameter optimization in this manuscript but since it was already being done for the other paper, Susiluoto et al., we decided to just refer to it. However, we agree this is now left too vague and as mentioned above, it is necessary to describe the optimisation in this manuscript also because there were some major differences between the approaches used here and in the final version of Susiluoto et al. We can add a new section in Materials and Methods that describes the parameter optimisation.

(5) Suggested changes to the manuscript:

We will add a new Section 3.2 (changing current 3.2 'Model testing' to 3.3) that describes the parameter optimization process done for this manuscript and remove references to Susiluoto et al. 2017 in, e.g. Table 1.

[As mentioned above, we changed the parameterization of the model completely. It is not anymore based on the study by Susiluoto et al. \(2017\) but on general literature values that are described in Section 3.2. Susiluoto et al. \(2017\) is a separate and more complete analysis on the significance of the parameters.](#)

(6) *The cited paper by Rinne et al. (2007) shows an exponential dependence of the measured flux on the peat temperature to day 200 (Figure 6 in paper). The lack of a temperature dependence presumably indicates that the temperature dependence is effectively determined by that of the input 'anaerobic carbon decomposition rate'. The temperature-dependence revealed in Fig. 6 is presumably associated with the modelled transport and loss processes.*

(6) Response:

Yes, this is correct. The temperature dependence in Fig 6 in our manuscript results from the impact of temperature to the processes simulated by HIMMELI, when its input respiration did not depend on temperature. Presumably the exponential dependence of CH₄ emissions on temperature would be observed if the anoxic respiration rate depended exponentially on temperature, which often is the case with soil respiration.

(6) Suggested changes to the manuscript:

We will emphasize this when discussing the Fig 6. (current p. 15).

We added a sentence emphasizing this issue, p. 19 l. 15-16.

(7) *Many of the key driving variables (soil temperature, leaf area index, water table depth) could be taken either from observations or modelled. It is not clear that this is the case for the anaerobic carbon decomposition rate. If it could be measured, this would improve the utility of HIMMELI.*

(7) Response:

This is true; direct measurement of the anoxic respiration rate is complex or impossible, it can be only estimated/simulated. Apparently the closest possible direct measurement would be on the CO₂ flux, which would require that the model includes simulation of photosynthesis, probably driven with solar irradiation. This would of course be possible, as we already now simulated photosynthesis (Appendix B) but our modelling work aimed at creating a module that takes anoxic respiration rate as input and thus is dependent on another model.

(7) Suggested changes:

-

(8) *The model is setup and the modelled CH₄ fluxes are compared to eddy covariance flux measurements of CH₄ made at Siikaneva, a peatland site in Southern Finland. The intake for the CH₄ flux measurements is given as 2.75 m above the peat surface (p. 13). Presumably the surface is fairly homogeneous as no information is given about the footprint nor the prevailing wind direction.*

(8) Response:

Siikaneva is a well-established site following the common standards and requirements for eddy-covariance measurements and its characteristics and representativeness of the data has been analyzed in several papers (Aurela et al. 2007, Rinne et al. 2007). The site is under ICOS (Integrated Carbon Observation System) labelling process to get accepted as an ICOS Class 2 site.

(8) Suggested changes to the manuscript:

We can add the information given above into the manuscript.

We added this, p. 16 l. 2-4.

(9) *A good fit of the observed and measured fluxes is seen over several annual cycles. This site is effectively used for both model calibration/optimisation and evaluation. This begs the question of how general the derived parameter values are or whether are they specific to this site. There is an obvious need for comparison against measurements from other sites.*

(9) Response:

The purpose of running the test with data from the Siikaneva site was principally to demonstrate that combined with realistic input, HIMMELI does output realistic CH₄ fluxes, which is not so evident if looking at the mechanistic sensitivity tests only. The parameter values are chosen to be physically sound and so they should, in principle, fit also other peatland sites but they are not given as general values for large-scale modelling. They were used here since they were optimized for the Siikaneva site. When moving to other peatlands and especially for large-scale modelling, the model needs to be recalibrated.

We agree that all this was left quite vague in the manuscript and that it would be interesting to see how well the current parameterisation fits to other peatland sites.

(9) Suggested changes to the manuscript:

We will define the scope of this part of the work and the validity of these parameter values better. In addition, we can add a comparison against 5 years of CH₄ flux measurements from another peatland site, Lompolojänkki, a subarctic fen site in Northern Finland (Aurela et al. 2009). This would be a test on how well the current parameterisation fits to another peatland site.

[We changed the parameterisation \(Sect. 3.2\), re-formulated Section 3.3.4 and added the comparison with fluxes from Lompolojänkki \(main additions are in Sects. 3.4., 4.4 and Appendix B\).](#)

(10) *It would have been interesting to see upscaled fluxes to the regional/boreal scale and hence an estimate of methane emissions from boreal peatlands.*

(10) Response:

This is certainly true, however, this is not within the scope of this paper. This will be done in future works when HIMMELI is combined with a large-scale land surface model.

(10) Suggested changes to the manuscript:

-

Technical comments:

(11) *The ellipsis (...) is used throughout the paper for 'to', e.g., page 12, line 14: '10...50 cycles' instead of '10 to 50 cycles'*

(11) Response:

The manuscript preparation guidelines of this journal say: "A range of numbers should be specified as "a to b" or "a...b". We chose to use "a...b" everywhere, however, we can change this.

(11) Suggested changes to the manuscript:

We leave the "a...b" expression only in tables but within the text change it to "a to b".

[This was done.](#)

(12) *Intercomparison is used in several places when 'comparison' is sufficient (a) Page 1, line 30; (b) Page 12, lines 20 and 22; (c) Page 17, line 18.*

(12) Response:

Agreed.

(12) Suggested changes to the manuscript:

We will change 'intercomparison' to 'comparison'.

[Done.](#)

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HIMMELI v1.0: Helsinki Model of MEthane buiLd-up and emIssion for peatlands

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Abstract. Wetlands are one of the most significant natural sources of methane (CH₄) to the atmosphere. They emit CH₄ because decomposition of soil organic matter in waterlogged anoxic conditions produces CH₄, in addition to carbon dioxide (CO₂). Production of CH₄ and how much of it escapes to the atmosphere depend on a multitude of environmental drivers. Models simulating the processes leading to CH₄ emissions are thus needed for upscaling observations to estimate present CH₄ emissions and for producing scenarios of future atmospheric CH₄ concentrations. Aiming at a CH₄ model that can be added to models describing peatland carbon cycling, we [developed-composed](#) a model called HIMMELI that describes CH₄ build-up in and emissions from peatland soils. It is not a full peatland carbon cycle model but it requires the rate of anoxic soil respiration as input. Driven by soil temperature, leaf area index (LAI) of aerenchymatous peatland vegetation and water table depth (WTD), it simulates the concentrations and transport of CH₄, CO₂ and oxygen (O₂) in a layered one-dimensional peat column.

30 Here, we present the HIMMELI model structure, [and](#) results of tests on the model sensitivity to the input data and to the description of the peat column (peat depth and layer thickness), and [demonstrate that HIMMELI outputs realistic fluxes](#)~~an~~ [intercomparison of the modelled and measured CH₄ fluxes at Siikaneva, a peatland flux measurement site in Southern Finland by comparing modelled and measured fluxes at two peatland sites](#). As HIMMELI describes only the CH₄-related processes, not the full carbon cycle, our analysis revealed mechanisms and dependencies that may remain hidden when testing CH₄ models connected to complete peatland carbon models, which is usually the case. Our results indicated that 1) the model is flexible and robust and thus suitable for different environments; 2) the simulated CH₄ emissions largely depend on the

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prescribed rate of anoxic respiration; 3) the sensitivity of the total CH₄ emission to other input variables, ~~LAI and WTD~~, is mainly mediated via the concentrations of dissolved gases, in particular, the O₂ concentrations that affect the CH₄ production and oxidation rates; 4) with given input respiration, the peat column description does not significantly affect ~~significantly~~ the simulated CH₄ emissions in this model version.

5 1 Introduction

Methane (CH₄) is an important greenhouse gas, atmospheric concentrations of which have increased by more than 250% since preindustrial times, inducing the second largest radiative forcing among well-mixed greenhouse gases (Myhre et al., 2013). Wetlands are the largest single natural CH₄ source to the atmosphere and their CH₄ emissions respond to changes in climatic conditions, which can be seen at global level (Bridgham et al., 2013; Turetsky et al., 2014). In order to upscale observed CH₄ fluxes and to produce realistic scenarios for the future atmospheric greenhouse gas concentrations, it is thus essential to know how wetland CH₄ emissions respond to climatic variables. Modelling these responses has been active in recent years (e.g. Wania et al., 2010; Riley et al., 2011; Melton et al., 2013; Schuldt et al., 2013; Grant et al., 2015).

Freshwater wetlands emit CH₄ from decomposition of soil organic matter because oxygen (O₂) concentrations in their water-saturated soils are low ~~and no alternative electron acceptors exist~~. Anoxic decomposition of soil organic matter is partly carried out by methanogenic microbes that produce CH₄, so the decomposition process releases both CH₄ and carbon dioxide (CO₂) (Nilsson and Öquist, 2009). Anoxia has also forced vascular wetland plants to develop techniques to get O₂ to their roots that extend to the inundated soil layers. For example, sedge species from genera *Carex* and *Eriophorum*, common in northern fen-type peatlands, have aerenchyma, special tissue with air-filled spaces that allows diffusion of O₂ from the atmosphere to the roots (Moog and Brüggemann, 1998). Some aquatic plants transport O₂ actively through the aerenchyma with pressurized through-flow (Brix et al., 1996). As a by-product, these mechanisms also transport CH₄ to the atmosphere (Morrissey et al., 1993; Brix et al. 1996). In addition to transfer via plants, CH₄ is known to be emitted from peatlands as ebullition, i.e. release of CH₄ bubbles into the atmosphere, and by diffusion through the peat column. CH₄ can also be consumed in the soil by methanotrophic bacteria that derive their energy by oxidizing CH₄ to CO₂.

The three transport mechanisms and the CH₄ oxidation have been implemented in many peatland models in which the peat column is divided into layers and physically based formulations simulate the carbon processes in them (see a review in Xu et al. 2016). Many of them have features adopted from previous models – for instance, the Walter and Heimann (1996, 2000) model of CH₄ production and emission is frequently utilized — but often the implementations include specific modifications. Some of the models also simulate the O₂ transport and the simulated O₂ concentrations affect the CH₄ processes. ~~This type of~~ these models have been used in multiple studies (e.g., Berrittella and van Huissteden, 2009, 2011; Khvorostianov et al., 2008; Ringeval et al., 2011; Melton et al., 2013; Budishchev et al., 2014; Cresto Aleina et al., 2015; Grant et al., 2015), and some

are referred to in the Assessment Report of the Intergovernmental Panel on Climate Change (IPCC; Ciais et al., 2013). These models have different approaches in simulating the production of CH₄, ranging from separating distinct heterotrophic microbial communities (Grant and Roulet, 2002) to taking a constant fraction of the simulated heterotrophic soil respiration (Riley et al., 2011). After that, the transport models essentially take care of determining which portion of the CH₄ is oxidized, and which is released to the atmosphere.

~~All existing soil carbon models do not yet include the simulation of peatland CH₄ emissions.~~ As CH₄ transport and oxidation can be simulated separately from other soil carbon processes, without the need to feed back to the main soil model, they can form a separate module. ~~There are soil models that simulate anoxic respiration (e.g., Clark et al., 2011; Schuldt et al., 2013) and so this would be their interface to a CH₄ module.~~ For this ~~kind of purposes~~, we ~~composed~~~~developed~~ HIMMELI, Helsinki Model of MEthane buiLd-up and emIssion, ~~which is a module that simulates only the processes related to transport and oxidation of CH₄.~~ It takes the rate of anoxic peat respiration as input, defined here as the rate of anoxic decomposition of organic compounds in peatland soil, and computes the subsequent CH₄ emission by simulating the transport and build-up of CH₄, O₂ and CO₂ in the soil, as well as the CH₄ oxidation rate that depends on the prevailing O₂ concentrations. HIMMELI is driven with soil temperature, water table depth and the leaf area index of the gas-transporting plant canopy.

~~HIMMELI does not bring any new processes as such into the CH₄ model world and it utilizes process descriptions largely adopted from earlier models (e.g., Arah & Stephen, 1998; Tang et al., 2010; Wania et al., 2010). However, it is among the most complete models considering the transport of compounds. According to Xu et al. (2016), there are only 5 models that simulate all vertically resolved biogeochemistry, O₂ availability to CH₄ oxidation, and three pathways of CH₄ transport. Of these, the Xu model (Xu et al., 2007), CLM-Microbe (Xu et al., 2014) and VISIT (Ito and Inatomi, 2012) do not explicitly simulate O₂ 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), *ecosys* (version in Grant and Roulet, 2002) and a recent model by Kaiser et al. (2017) – not included in the list by Xu et al. (2016) – do simulate all these. HIMMELI also simulates CO₂ transport via all three transport pathways. This is not a common feature in CH₄ models: to our knowledge, only the multi-substance version of TEM (Tang et al., 2010), *ecosys* (Grant and Roulet, 2002) and the Segers model (Segers and Leffelaar, 2001) included that. The novelty of HIMMELI is that it has been developed independent of a full peatland carbon model, with the ambition to obtain a robust and flexible model that can be easily used as a tool within different environments as, for instance, its peat column structure is not fixed.~~

~~It uses process descriptions largely adopted from earlier models, but the novelty is that it has been developed independent of a full peatland carbon model, with the ambition to obtain a robust and flexible model that can be easily used as a tool within different environments.~~ Sensitivity analyses on the complete peatland models have been presented, mostly concentrating on the sensitivity to model parameters (e.g. Berrittella and Huissteden, 2009, 2011; Tang et al. 2010; Wania et al., 2010; Zhu et

al., 2014), but we are not aware of any studies which would have analyzed the sensitivity of the CH₄ models as such to driving variables. This kind of analysis is, however, important because a CH₄ module can form a considerable part of a peatland carbon model and studying it alone may reveal dependencies that affect the output CH₄ emissions but are not seen in sensitivity tests on full carbon models. Because HIMMELI includes components similar to earlier CH₄ models, the results of the sensitivity analysis should be interesting for the modeling community.

In the present work, we a) define key factors for CH₄ transport and oxidation, b) describe the model, c) analyze its dynamics and sensitivity of output fluxes to input data in steady-state tests, d) analyze the model sensitivity to the description of the peat column by running the model for a Finnish peatland flux measurement site Siikaneva (Rinne et al., 2007), and e) demonstrate with data from Siikaneva and another site Lompolojänkki (Aurela et al., 2009) that combined with realistic input, HIMMELI output CH₄ fluxes are realistic compared to measurements, which is not so evident if looking only at the mechanistic sensitivity tests. evaluate the model against measured CH₄ fluxes at Siikaneva.

2 Key factors for CH₄ transport and oxidation

The rate of CH₄ production in peat has been found to be controlled by peat and substrate quality, temperature and pH (Valentine et al., 1994; Bergman et al., 1999; Reiche, 2010). However, the final emissions depend on how much CH₄ is consumed by methanotrophic bacteria. This can be up to 100% of the CH₄ produced (Whalen, 2005; Fritz et al., 2011). The probability of a CH₄ molecule to get oxidized is thought to depend on which pathway it takes to escape from the soil since the conditions are suitable for methanotrophy mostly in oxic peat layers. Ebullition may bypass this oxidative zone (Coulthard et al., 2009) and although methanotrophs are also found in some wetland plant roots (King, 1994), oxidation can largely be avoided by moving through the plants. Several studies have shown that the CH₄ emissions decrease clearly when the gas-transporting plants are removed from a site, indicating that aerenchymatous vegetation is an effective transport route for CH₄ (Waddington et al., 1996; King et al., 1998; Green and Baird, 2012).

Roots of sedges, particularly those of *Carex* species, extend deep to the soil (Shaver and Cutler, 1979; Saarinen, 1996). Therefore they have a large contact surface with the anoxic peat. The area of root surface permeable to gases was the most important factor controlling the CH₄ flux in *Juncus effusus*, another aerenchymatous species, and this permeable surface is concentrated in fine roots and the tips of coarser roots (Hennenberg et al., 2012). According to Reid et al. (2015), the rate for root-mediated gas transport in *P. australis* and *Spartina patens* increased during the growing season, indicating increase of permeable root surface area or aerenchyma along the summer. Thus, the growth of the plants seems to affect their gas transport capacity. Isotopic studies have shown that passive diffusion down the concentration gradient dominates the CH₄ transport in sedges (Chanton and Whiting, 1993; Popp et al., 1999), and Moog and Brüggemann (1998) also demonstrated that diffusion is a sufficient explanation for the supply of O₂ to the roots of *Carex* species. There are, however, contrasting findings about

where the main resistance for the diffusive CH₄ flux lies. Kelker and Chanton (1997) suggested it is belowground, at the soil-root or root-shoot boundary, and that *Carex* releases CH₄ not through the leaf blades (and stomata) but from the point where the leaves bundle. This would be similar to rice (*Oryza sativa*), *Menyanthes trifoliata* and *J. effusus* that release CH₄ from the stem or leaf sheath, possibly through micropores, not stomata (Nouchi et al., 1990; Macdonald et al., 1998; Hennenberg et al., 2012). However, in the studies by Schimel (1995) and Morrissey et al. (1993), CH₄ seemed to exit the sedges through the leaf blades and stomata and this would thus form the main resistance for the flux in the plant. Diurnal variation of the CH₄ emissions could indicate stomatal control but clear diurnal patterns have not been observed (Rinne et al., 2007; Jackowicz-Korczyński et al., 2010), the maximum emissions may even occur at night (Mikkilä et al., 1995; Waddington et al., 1996; Juutinen et al., 2004). On the other hand, possible diurnal changes in O₂ diffusion to the rhizosphere may be reflected in the CH₄ fluxes since O₂ concentration affects the rate of CH₄ oxidation (Thomas et al., 1996), as well as diurnal changes in the CH₄ substrate input from the photosynthesizing vegetation may affect CH₄ production (Mikkilä et al., 1995).

Gas ebullition occurs, in principle, when the concentration of a dissolved gas reaches saturation, but in practice, CH₄ ebullition has been observed in wetlands already with concentrations below saturation (Baird et al., 2004; Kellner et al., 2006; Waddington et al., 2009; Bon et al., 2014). Other gases increase the gas pressure and soil particles and impurities lower the energy barrier for gas nucleation. The CH₄ content in ebullitive gas fluxes has been estimated to be 45% to 60% (Glaser et al., 2004; Tokida et al., 2005; Kellner et al., 2006) and the rest consists mainly of O₂, CO₂ and nitrogen (N₂) (Tokida et al., 2005). The volumetric gas content (VGC) in the peat has been observed to be approximately 10% to 15% (Kellner et al., 2006; Tokida et al., 2007; Waddington et al., 2009) indicating that all the formed gas does not escape the soil. Ebullition events seem to be affected by atmospheric pressure. When the pressure declines, bubble volume increases and the solubility of gases decreases allowing more gases to accumulate in the bubbles, consequently, their buoyancy may overcome the forces that resist their movement and ebullition occurs (Tokida et al., 2007; Waddington et al., 2009). Increasing pressure, by contrast, may enhance the bubble mobility through the peat by causing bubble size to decrease (Comas et al., 2011). Movement of bubbles also depends on the peat structure that varies along the peat column as well as within and between peatlands, due to differences in peat composition and decomposition status (Rezanezhad et al., 2016). The shallow, less decomposed peat has more space for the bubbles, while the more decomposed deeper peat layers are tighter packed (Comas et al., 2011).

Properties of the peat column also affect the diffusion of CH₄ and O₂ in the air- and water-filled peat pores. Porosity of the soil, i.e., the fraction of the soil volume that is taken up by the pore space, as well as interconnectivity, pore shape and size distribution determines the rate of diffusion; ~~the lower it is, the slower is diffusion~~. Different descriptions of the dependency of diffusion coefficient on the soil porosity or tortuosity have been presented (Millington, 1959; Collin and Rasmuson, 1988; Staunton, 2008). The porosity of peat soils is generally high, at least 80% (Mitsch and Gosselink, 2007). Therefore, peat does not hinder the diffusion as much as many other soil types. In models the peat column is commonly considered in a simplified way, assuming that the water table depth (WTD) forms a border below which the peat is saturated with water and above which

peat pores are air-filled. However, in reality the division is not this strict as VGC can be a considerable fraction of the total volume below the WTD for instance, due to the gas production in the peat (Waddington et al., 2009), and the peat can be wet above the WTD if the peat pores retain water when the WTD drops (Estop-Aragonés et al., 2012; Fan et al., 2014). Diffusion through the peat column is thought to be a minor component in the total CH₄ emissions of a peatland when gas-transporting vegetation is present at the site (Walter et al., 1996; Lai, 2009), because the diffusion coefficient in water is approximately 4 orders of magnitude lower than in gas (Staunton, 2008) and because the probability of CH₄ being consumed by methanotrophs is higher in the peat, especially when the WTD is low (Estop-Aragonés et al., 2012).

Methanotrophic bacteria occur in all soils, not only wetlands, and methanotrophy in upland soils is the largest biogenic sink of atmospheric CH₄ (Ciais et al., 2013). Rate of the CH₄ oxidation reaction depends on the concentrations of both CH₄ and O₂ (Watson et al., 1997) and since CH₄ oxidation is a biochemical reaction, the rate is also limited by factors that affect the microbial activity, such as temperature (Whalen and Reeburgh, 1996). When the WTD is low, the O₂ concentrations in the top peat layers are high favoring CH₄ oxidation (Moore et al., 2011; Estop-Aragonés et al., 2012). However, there can be anoxic areas above the WTD (Silins and Rothwell, 1999; Fan et al., 2014) and the O₂ transported down by plant roots provides conditions suitable for methanotrophy also in the inundated peat layers (Fritz et al., 2011).

3 Model and methods

3.1 Model description

3.1.1 General

The model (Fig. 1) simulates microbial and transport processes that take place in a one-dimensional peat column, keeping track on the concentration profiles of CH₄, O₂ and CO₂. The output is fluxes of CH₄, O₂ and CO₂ between the soil and the atmosphere, with the possibility to separate the contributions of the three different transport routes, as well as to extract the amount of oxidized CH₄. The required input and the model output is explained in more detail within the model code package that is provided as a Supplement of this article. So far the model does not consider freezing and ice, but it is valid when peat water is not frozen. Parameter values used in the present study (Table 1) were based on literature values (see Section 3.2) and the aim was to have physically sound parameter values. However, if using HIMMELI in large-scale CH₄ modeling, the model possibly needs to be re-calibrated.

The model is driven with:

- peat temperature, T (K)
- leaf area index of aerenchymatous gas-transporting vegetation, LAI (m² m⁻²)
- water table depth, WTD (m)

- anaerobic carbon decomposition rate, i.e., the rate of anoxic respiration for the area of the peatland, V_{anR} ($\text{mol m}^{-2} \text{s}^{-1}$).

Parameter values used in the present study are listed in Table 1. Some of them were taken directly from earlier literature (Arah and Stephen, 1998; Vile et al., 2005), but a set of parameter values was obtained by optimizing with Bayesian methods with respect to fluxes measured at the Siikaneva peatland site (see Sect. 3.3) using a least squares objective function with the adaptive Metropolis Markov chain Monte Carlo method (Haario et al., 2001). The values used are the best estimate of these values, i.e., the parameter set of the lowest negative log likelihood. The uncertainty of some of these parameters is rather high, and a more complete analysis can be found in Susiluoto et al. (2017, *in prep.*).

The reaction-diffusion equations governing the concentrations of the three compounds CH_4 , O_2 and CO_2 at depth z are (Eq. 1-3):

$$\frac{\partial}{\partial t} C_{\text{CH}_4}(t, z) = -\frac{\partial}{\partial z} F_{\text{CH}_4} - Q_{\text{plt}, \text{CH}_4} - Q_{\text{ebu}, \text{CH}_4} + R_{\text{CH}_4} - R_O \quad (1)$$

$$\frac{\partial}{\partial t} C_{\text{O}_2}(t, z) = -\frac{\partial}{\partial z} F_{\text{O}_2} - Q_{\text{plt}, \text{O}_2} - Q_{\text{ebu}, \text{O}_2} - R_{aR} - 2R_O \quad (2)$$

$$\frac{\partial}{\partial t} C_{\text{CO}_2}(t, z) = -\frac{\partial}{\partial z} F_{\text{CO}_2} - Q_{\text{plt}, \text{CO}_2} - Q_{\text{ebu}, \text{CO}_2} + (R_{anR} - R_{\text{CH}_4}) + R_O + R_{aR} \quad (3)$$

Here, F_{CH_4} , F_{O_2} , and F_{CO_2} are the diffusive fluxes in the peat (in water below the WTD and in air above it; see Sect. 3.1.8), $Q_{\text{plt}, X}$ and $Q_{\text{ebu}, X}$ are the transport rates of gas X between peat and atmosphere via plant roots and by ebullition, respectively, R_{CH_4} is CH_4 production rate, R_{anR} is the rate of anaerobic respiration, R_{aR} is the rate of aerobic respiration and R_O is the CH_4 oxidation rate.

The ~~current set-up of the model~~ has been developed principally using a daily timestep for input and output, as our main target has been to use it with models that provide daily input. ~~runs in one day resolution, taking the~~ However, we also tested running HIMMELI on a shorter timestep (Sect. 3.3.2) input as daily averages. ~~The differential equations are solved simultaneously using the fourth order Runge-Kutta method.~~ The internal time step is determined by the turnover time of CH_4 and O_2 concentrations in the peat. It is assumed that the longest usable time step is half of the turnover time. The differential equations are solved simultaneously using the fourth order Runge-Kutta method.

3.1.2 Peat geometry, root distribution and movement of water

The model basically describes a one-dimensional vertically layered peat column. Peat depth and layer thicknesses are not fixed but different set-ups can be used. The only limitation for the layer structure is that if the peat thickness exceeds 2 m, there has

to be a layer border exactly at the 2 m depth, because of how the roots are treated in the model. The layering below 2 m must start from that depth.

In the model, WTD is a strict divider of the peat into water-filled and air-filled parts. This has been implemented by adding an extra layer in the pre-described layer composition (Fig. 1). Its thickness is adjusted so that the water surface is always exactly at the interface between the two layers. This approach enables using the exact given WTD as input. Only in the case that the boundary of the extra layer would be closer than 1 cm to a boundary of the background layering, the WTD is rounded to this nearest permanent layer boundary. Strict division of the peat to air-filled and water-filled parts is a simplification since anoxic sites can occur above the WTD (Estop-Aragonés et al., 2012). However, as in site-level and larger scale simulations even an observation-based WTD is an approximate value over peatland areas, we consider the strict division to anoxic and oxic parts a robust approach.

In HIMMELI, the water level can also be above the peat surface and in this case ~~an~~the extra water layer is located above the peat surface. In nature, windmixing can affect the concentrations of different compounds in free water but this is not considered in the model. This simplification is justified as there often is vegetation that decreases the windmixing via affecting wind speed.

Changing WTD essentially means addition or removal of water to/from the peat column. At the same time, the masses of CH₄, O₂ and CO₂ need to be conserved. In the case of rising WTD, the CH₄, O₂ and CO₂ that were in the air-filled layers are dissolved in the water until the concentrations in the newly water-filled layers reach the solubility limit with the previous air concentrations. The excess gas is pushed upwards to the lowest air-filled layer (or to the atmosphere). In the case of lowering WTD, the CH₄, O₂ and CO₂ of the previously water-filled layers are introduced into the air-filled layers replacing them. This can cause ~~abnormally~~ exceptionally high or low fluxes and concentrations in some layers, but these even out fast in relation to the daily time step, mainly through diffusion.

An essential role is played by the vertical distribution of plant roots since that determines how the input anoxic respiration and the gas-transporting root mass is distributed vertically. The formulation has been adopted from Wania et al. (2010):

$$f_{root}(z) = C e^{-z/\lambda} \quad (4)$$

where $f_{root}(z)$ is the fraction of roots at depth z , λ is a root depth distribution decay parameter and C is a normalizing constant defined so that the sum of root fractions equals 1 (Eq. 5):

$$\int_0^{z_{max}} f_{root}(z) dz = 1. \quad (5)$$

The maximum depth that the roots are assumed to reach is 2 m (Saarinen, 1996). If the peat depth exceeds 2 m there is a rootless zone at the bottom. The value of C depends on the peat thickness and geometry of the current peat column and it is calculated at each time step, so the root distribution can adjust to changing peat depth.

3.1.3 CH₄ production

- 5 ~~Since root exudates are an important carbon source for the methanogens,~~ The input anaerobic respiration (V_{anR}) is distributed vertically along the root distribution in the anaerobic peat layers below the WTD (Eq. 6):

$$R_{anR}(z) = \frac{V_{anR}}{dz} f_{root,an}(z) . \quad (6)$$

- Here $R_{anR}(z)$ (mol m⁻³ s⁻¹) is the rate of anoxic respiration at depth z , $f_{root,an}(z)$ refers to the ratio of root mass at depth z to the total root mass of the anaerobic zone and dz (m) is the layer thickness. In the case that peat depth exceeds the maximum rooting depth 2 m, the model calculates what would be the anaerobic respiration rate at the bottom root layer if all the input carbon was allocated in the rooting zone, then allocates 50% of that in the rootless layers, and the remainder is re-distributed to the rooting zone.

- 15 This choice of distributing the anoxic respiration with root mass (as opposed to distributing it e.g. evenly across the peat column) was motivated by the fact that recently fixed carbon, such as root exudates, seems to be the main source of CH₄. For instance, according to Oikawa et al. (2017), less than 5% of CO₂ and CH₄ emissions originate from soils below 50 cm in flooded peatlands. However, in case that HIMMELI is used in a study where it is essential to simulate the different carbon sources and distribute CH₄ production in a different way, it is relatively easy to modify the code so that this becomes possible.

- 20 CH₄ production rate R_{CH4} (mol m⁻³ s⁻¹) in a peat layer at depth z is calculated as a fixed fraction (f_m) of R_{anR} but the rate may be inhibited by dissolved O₂, following Arah and Stephen (1998) (Eq. 7):

$$R_{CH4}(z) = f_m R_{anR}(z) \frac{1}{1 + \eta C_{O2}(z)} , \quad (7)$$

- where η is a parameter reflecting the sensitivity of methanogenesis to O₂ inhibition. The CH₄ production rate in conditions with no O₂, i.e., C_{O2} is zero, is called potential methane production (PMP) in this paper. The rest of the anaerobic respiration ($R_{anR} - R_{CH4}$) produces CO₂. HIMMELI does not include electron acceptors other than O₂

- ~~In the case that peat depth exceeds the maximum rooting depth 2 m, the model calculates what would be the anaerobic respiration rate at the bottom root layer if all the input carbon was allocated in the rooting zone, then allocates 50% of that in the rootless layers, and the remainder is re-distributed to the rooting zone.~~ since their concentrations can be expected to depend on site characteristics, it would thus be difficult to estimate them and these estimates would not necessarily improve the

accuracy of the model. However, including known factors that affect CH₄ production, such as the alternative electron acceptors, is important and could possibly be a way to take into account site differences in future model versions.

3.1.4 Aerobic respiration

- 5 All the O₂ in the peat is not consumed by the methanotrophs but other aerobic microbe processes like aerobic peat respiration also require O₂. This O₂ consumption rate that affects the O₂ availability of CH₄ oxidation is estimated with a Michaelis-Menten model, following Arah and Stephen (1998) (Eq. 8):

$$R_{aR}(z, T) = V_R(T) \frac{c_{O_2}(z)}{K_R + c_{O_2}(z)}, \quad (8)$$

- 10 where R_{aR} (mol m⁻³ s⁻¹) is the rate of aerobic respiration at temperature T at depth z, V_R (mol m⁻³ s⁻¹) is the potential rate of respiration at temperature T, and K_R (mol m⁻³) is the Michaelis constant for the reaction. This reaction produces 1 mol of CO₂ per each mol of O₂ consumed.

3.1.5 CH₄ oxidation

Rate of CH₄ oxidation is assumed to follow the dual-substrate Michaelis-Menten kinetics (Arah and Stephen 1998) (Eq. 9):

$$R_O(z, T) = V_O(T) \frac{c_{O_2}(z)}{K_{O_2} + c_{O_2}(z)} \times \frac{c_{CH_4}(z)}{K_{CH_4} + c_{CH_4}(z)}, \quad (9)$$

- 15 where R_O (mol m⁻³ s⁻¹) is the oxidation rate at temperature T at depth z, V_O (mol m⁻³ s⁻¹) is the potential oxidation rate at temperature T, K_{O_2} (mol m⁻³) and K_{CH_4} (mol m⁻³) are the Michaelis constants for O₂ and CH₄, respectively. Each CH₄ mol oxidized consumes 2 moles of O₂ and produces 1 mol CO₂.

3.1.6 Temperature dependency of microbial reactions

- 20 The reaction rates of oxidation and aerobic respiration depend on temperature following the form of the Arrhenius equation (Eq. 10):

$$V(T) = V_\theta \exp\left(\frac{\Delta E}{R} \left(\frac{1}{T_\theta} - \frac{1}{T}\right)\right), \quad (10)$$

where $V(T)$ refers here to the rate of oxidation or aerobic respiration at temperature T, V_θ (mol m⁻³ s⁻¹) is the reaction rate at the reference temperature T_θ (K), R (J mol⁻¹ K⁻¹) is the gas constant and ΔE (J mol⁻¹) the activation energy of the reaction.

3.1.7 Ebullition

- 25 The ebullition model takes into account concentrations of CH₄, CO₂, O₂ and N₂ and uses the sum of their partial pressures to determine when ebullition occurs. This approach was previously used by Tang et al. (2010). In HIMMELI, ebullition is the

only process that takes N_2 into account. We assume N_2 is always in equilibrium with the atmospheric concentration and so its partial pressure in the peat is always 78% of the atmospheric pressure. The model computes the solubilities of CH_4 , CO_2 and O_2 in water using the dimensionless Henry's law coefficient (see Appendix A for formulation; Sander, 2015).

- 5 If the sum of the partial pressures pp (Pa) of the dissolved CH_4 , CO_2 , O_2 and N_2 (pp_X) exceeds the sum of the atmospheric and hydrostatic pressures (P_{atm} and P_{hyd} , respectively) (Eq. 11):

$$\sum_X pp_X(z) > P_{atm} + P_{hyd}(z) \quad (11)$$

ebullition occurs. The model first computes the fraction of ebullition, f_e (Eq. 12):

$$f_e(z) = \frac{\sum_X pp_X(z) - (P_{atm} + P_{hyd}(z))}{\sum_X pp_X(z)} \quad (12)$$

- 10 and this fraction of each gas is removed, expressed as a rate by introducing time constant k (s^{-1}) in the equation. ~~The value of k was chosen for numerical reasons to be $1/1800$ s, which ensures the half life of the gas is larger than the internal time step.~~ The ebullition ~~flux-rate~~ $Q_{ebu,X}$ ($mol\ m^{-3}\ s^{-1}$) of compound X from a soil layer at depth z thus is (Eq. 13):

$$Q_{ebu,X}(z) = -k \frac{f_e(z) pp_X \sigma}{RT}, \quad (13)$$

- 15 where σ is peat porosity. Ebullition only occurs in the water-filled peat. If the WTD is below the peat surface, the ebullited gases are transferred into the lowest air-filled soil layer and they continue from there via diffusion in the peat or in plant roots. Otherwise the ebullition is released directly into the atmosphere.

- 20 In reality, bubble movement in porous media is a highly complex problem that depends on the fine-scale structure of the media. After a bubble has been formed there are several processes that take place before the bubble reaches the surface and contributes to the CH_4 flux to the atmosphere. For instance, the bubbles need to traverse through the peat column and on the way they interact with the surrounding pore water and hence alter the CH_4 concentration gradients. These processes are still missing from most of the peatland CH_4 models (Xu et al., 2016), including HIMMELI. This is most likely because relatively little is known about bubble movement in peat and how to describe it accurately in models, although there are some attempts to model this process (Ramirez et al., 2015). Different ebullition modelling approaches were compared by Peltola et al. (2017).

25 3.1.8 Diffusion in the peat

Simulation of diffusion in the porous water-filled or air-filled peat takes into account the reduction in the diffusivity compared with pure water or air (see e.g. Iiyama and Hasegawa, 2005). The diffusion coefficients used in this study are listed in Appendix A. The effective diffusivities in the porous peat ($D_{peat,w}$ and $D_{peat,a}$; $m^2\ s^{-1}$) are calculated by multiplying the free-water or free-

air diffusivities by (dimensionless) constant reduction factors $f_{D,w}$ and $f_{D,a}$ ~~whose values were derived from the optimization (Susiluoto et al., 2017)~~ (Eq. 14 and 15).

$$D_{peat,w} = f_{D,w}D_w \quad (14)$$

$$D_{peat,a} = f_{D,a}D_a \quad (15)$$

- 5 The diffusion (F_X ; mol m⁻² s⁻¹) of compound X between layers is calculated using a difference equation that is set up between the centre points ($i-1$ and i) of the layers (Eq. 16):

$$F_{i-1,i} = D_{peat,X} \frac{(C_{X,i-1} - C_{X,i})}{dx} \quad (16)$$

Here dx (m) is the distance between points $i-1$ and i and $C_{X,i-1}$ and $C_{X,i}$ are the concentrations at these layers. The surface layer at the water-air interface is assumed to be in equilibrium with the gas phase concentrations according to the Henry's law. The diffusion flux across the water-air interface is then calculated from the difference in concentration between the layer centre points and water-air interface as shown by Bird et al. (1960). The final equation for the flux of compound X at the interface becomes (Eq. 17):

$$F_X = \frac{2D_{peat,w}D_{peat,a}C_{X,w} - k_{H,X}C_{X,a}}{D_{peat,a} + D_{peat,w}k_{H,X}} \quad (17)$$

- where $D_{peat,w}$ and $D_{peat,a}$ are the diffusion coefficients in the water and air-filled layers, $k_{H,X}$ is the Henry's law coefficient in dimensionless form (Appendix A) and $C_{X,w}$ and $C_{X,a}$ (mol m⁻³) are the concentrations of compound X in the water-filled and air-filled layer, respectively.

3.1.9 Plant transport

- Formulation of plant transport ~~flux rate~~ $Q_{plt,X}$ of compound X (mol m⁻³ s⁻¹) is similar to many other peatland models in that it describes diffusion in air-filled tubes that represent aerenchymatous plant roots. We employ the formulation from Stephen et al. (1998) that uses the density of cross-sectional area of root endings as the variable expressing the abundance of gas-transporting vegetation (Eq. 18):

$$Q_{plt,X}(z) = \frac{\varepsilon_r(z)D_{peat,a}C_X(z,t) - C_{atm,X}}{\tau} \quad (18)$$

- Here ε_r is the density of cross-sectional area of root endings at depth z (m² m⁻³) and τ is root tortuosity. To account for the porous structure of aerenchyma (Colmer, 2003), HIMMELI uses the same value as in air-filled peat, $D_{peat,a}$ (m² s⁻¹), as the diffusion coefficient inside roots. It is averaged over the temperatures of the different layers between each depth z that the roots go through. ε_r follows the root distribution and it depends on the LAI of the vegetation via (Eq. 19):

$$\varepsilon_r(z) = a_{mA} \frac{f_{root}(z) LAI}{A \times dz SLA} \quad (19)$$

where a_{mA} expresses the cross-sectional area of root endings per root dry biomass ($\text{m}^2 \text{kg}^{-1}$), A is the area of the peat layer (m^2), dz is the layer thickness (m) and SLA is the specific leaf area ($\text{m}^2 \text{kg}^{-1}$). Root mass is thus assumed to equal the aboveground biomass.

5 3.2 Model parameterization

Table 1 lists the parameter values used in this study, as well as the literature reference of cases where the value was taken directly from one study. Here we go through the parameter values that were based on several papers or some calculation. The parameterization of HIMMELI has been analyzed in more detail in a separate study by Susiluoto et al. (2017).

- 10 The CH_4 oxidation model has four parameters: K_{O_2} , K_{CH_4} , V_O and ΔE_O . Watson et al. (1997) used K_{O_2} of 0.032 mol m^{-3} and we chose to use this value rounded to 0.03 mol m^{-3} . For K_{CH_4} we found several literature values: 0.001 mol m^{-3} in Dunfield et al. (1993), 0.045 and 0.058 in Watson et al. (1997), and 0.001 to 0.045 in the review by Segers (1998). We chose an average of these, i.e., 0.03 mol m^{-3} . Dunfield et al. (1993) found that the activation energy of methanotrophy is 20 to 80 kJ mol^{-1} and also here we chose the average, 50 kJ mol^{-1} . Using this in the Arrhenius equation (Eq. 10) fitted well with the V_O values reported
- 15 by Watson et al. (1997) and Dunfield et al. (1993) that were $28 \mu\text{mol m}^{-3} \text{ s}^{-1}$ at 25°C and 12 to $15 \mu\text{mol m}^{-3} \text{ s}^{-1}$ at 15°C , respectively and thus we set V_O to $10 \mu\text{mol m}^{-3} \text{ s}^{-1}$ at the reference temperature T_σ , 283 K .

- The model of aerobic respiration has three parameters: K_R , V_R and ΔE_R . Watson et al. (1997) used K_R of 0.022 mol m^{-3} and Iiyama et al. (2012) found in their review a K_R range of approximately 0.002 to 0.02 mol m^{-3} . On this basis, we set this to 0.02
- 20 mol m^{-3} . Stephen et al. (1998) used ΔE_R value of 50 kJ mol^{-1} , which was supported by Lloyd and Taylor (1994), hence, we also used this value for the activation energy. V_R was based on observed respiration rates on the Siikaneva peatland measurement site (Sect. 3.4.1) that we used in model testing. Respiration rate derived from the mean temperature, mean WTD and mean CO_2 emission rate observed in July 2005 at Siikaneva (Aurela et al., 2007) was $16 \mu\text{mol m}^{-3} \text{ s}^{-1}$ at 16.5°C . Using the ΔE_R mentioned above in Eq. 10, V_R at the reference temperature T_σ 283 K was approximately $10 \mu\text{mol m}^{-3} \text{ s}^{-1}$.

- 25 Fraction of anaerobic respiration becoming CH_4 , f_m , affects CH_4 generation and therefore also the emission rate directly. According to Nilsson and Öquist (2009), theoretically the CH_4 yield from terminal mineralization of soil organic matter in optimal methanogenic conditions ranges from 0 to 70% , being around 50% when carbohydrates are mineralized. Their literature review showed, however, dominance of CO_2 : the observed CO_2/CH_4 quotient in anoxic incubations had varied from

0.5 to 36,000 with median value in a filtered data set being around 6. HIMMELI does not simulate different CH₄ production pathways or methanogen groups but uses only this one parameter. We chose to use the conservative ratio 50/50, i.e. f_m of 0.5.

Peat porosity σ was based on the review by Rezanezhad et al. (2016) that gave a range 71 to 95%. We chose to use an average value 85%. Reduction factors for the water and air diffusion coefficients in peat, $f_{D,w}$ and $f_{D,a}$, were set by using the model by Millington and Quirk (1961) (Eq. 20):

$$\frac{D_S}{D_0} = \sigma^{\frac{3}{4}} \quad (20)$$

where D_S is the diffusion coefficient in soil and D_0 in free air. The resulting reduction factor was 0.80. We do not know to what extent this applies also to diffusion in water, however, we used the same value for both $f_{D,w}$ and $f_{D,a}$.

SLA values for graminoids or sedges varied widely in literature. Raivonen et al. (2015) found that the SLA of sedges in one peatland site was 7 m² kg⁻¹, Poorter and De Jong (1999) reported the SLA of *Carex* species on a fen to be on average 15 m² kg⁻¹, and Vile et al. (2005) gave 23 m² kg⁻¹ generally for graminoids. We decided to use an average, 15 m² kg⁻¹. Time constant for ebullition, k , was set to 1/1800 s based on model numerics, now the half-life of the excess concentrations becomes longer than the usual internal time step.

3.3 Model testing

We analyzed HIMMELI's sensitivity to the driving input variables, length of time step, and to the description of the peat column, i.e., peat column depth and layer thickness. The model sensitivity to input variables and time step length ~~former~~ was analyzed using steady-state tests and transition tests (see Sections 3.2.3.1 and 3.3.2). ~~and~~ The effect of the peat column set-up was analysed ~~later~~ by ~~simulating~~ running HIMMELI with data from the Siikaneva peatland site with different peat column descriptions (Section 3.2.4.2). In addition, we compared the modelled ~~and measured~~ CH₄ fluxes ~~to measured fluxes~~ at Siikaneva ~~and at another peatland site, Lompolojänkä~~ and conducted a rough evaluation of the model's ability to predict the observed CH₄ emissions (Section 3.4.2.2.3), in order to demonstrate that when combined with realistic input, HIMMELI outputs realistic CH₄ fluxes.

3.2.3.1 Testing model sensitivity to input data

The steady-state tests were conducted to study how sensitive the model is to the input data and to understand how the sensitivity depends on the modelled processes. We tested the model by running it into equilibrium with several different input value combinations, starting from empty concentration profiles of all the compounds. Specifically, we tested the sensitivity of the model to peat temperature, WTD, LAI (and corresponding root mass) and rate of anoxic respiration, by varying these one by

one. Temperature was always constant throughout the soil profile in these experiments, unlike in the simulations of the peatland Siikaneva sites.

We also conducted ~~two~~three transition tests to study the model response to changing WTD, temperature and anoxic respiration rate. In those, the model was first equilibrated with one set of driver values and after that the WTD, peat temperature or anoxic respiration was alternated. The different input combinations, details of the tests and their names are summarized in Tables 2 and 3.

The tests are ~~named~~labelled so that the first letter (T for temperature, W for WTD, L for LAI and R for respiration) tells which input varied and the rest shows the values of the constant input variables, with the simplification that W03 stands for WTD of -0.3 m. The transition test names just show the changing variables; Wtr stands for WTD transition, Ttr for temperature transition and Rtr for respiration transition. The input range for LAI was based on, e.g., Slevin et al. (2015) and range of anoxic respiration on, e.g., Scanlon and Moore (2000) and Szafranek-Nakonieczna and Stepniewska (2014).

~~In these tests we used a value of 0.5 for the parameter f_m (Table 1), the fraction of anaerobic respiration converted to CH_4 , which was different from the value used for Siikaneva (0.25; see Sect. 3.2.2). However, this parameter practically only controls the output CH_4 emission levels, and its effects on the model dynamics are minor.~~

In these mechanistic sensitivity tests, the anoxic respiration rate ($\text{mol m}^{-2} \text{s}^{-1}$) was independent of temperature and WTD since the purpose was to analyze the sensitivity of the processes that HIMMELI simulates, and anoxic respiration is only input for HIMMELI. We did not want to set any dependency here 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 kept the tests more generic. The idea was to analyze how much and via what pathways the other driving variables (WTD, temperature, LAI) affect the output CH_4 emission rate when the carbon input rate is constant. The input respiration was always allocated only to the inundated peat layers. Consequently, when the WTD varied, also the number of layers into which the anoxic respiration was allocated varied, although the total respiration rate of the peat column remained constant. ~~Temperature was always constant throughout the soil profile in these experiments, unlike in the simulations of the Siikaneva site.~~

3.3.2 Testing a time step of 30 min

In order to find out whether eliminating the diurnal temperature variation with the daily time step affects the modelled fluxes we compared a model run done on 30 min time step to a run done on the daily time step. We chose an arbitrary summer day, 1 July 2006, and took the soil and air temperature data measured at Siikaneva at 30 min intervals. All other input values were constant over the day in both runs. To avoid possible complications originating from the fact that the first and last temperatures of the chosen day differed by 3 degrees (air) and 0.5 degrees (top soil layer) we modified slightly the temperatures measured in the evening. We interpolated new values between the high afternoon temperatures and the new last temperature that was set

to be close to the first measurement of the day (Fig. 2). We ran HIMMELI over 35000 days using first these data and a 30 min time step, then using the daily average of the temperatures and a 24-h time step. Within this time, the concentrations reached reasonable saturation. WTD was set to -16 cm, the daily average WTD measured at Siikaneva on 1 July 2006, LAI was $1 \text{ m}^2 \text{ m}^{-2}$, and anoxic respiration rate was $1 \mu\text{mol m}^{-2} \text{ s}^{-1}$.

5 **3.23.23 Testing model sensitivity to the description of the peat column**

We ran the model with a seven-year input data series from the Siikaneva fen (see Sect. 3.3 and App. B) and tested how sensitive the results are to peat depth and peat layer thicknesses. We used the same input anoxic respiration, WTD and LAI for all the model runs. The only factor that changed slightly between the different set-ups was the soil temperature since the interpolated temperature profile always followed the layering. In these simulations, anoxic respiration was not constant but simulated (see App. B). The model spin-up was conducted by running the model through the entire seven-year time series of input data until the peat CH_4 concentrations stabilized. The spin-up time we used depended on the peat thickness, being ~~10...50~~ up to 600 cycles in the case of 5 m peat.

We tested four peat depths, 1 m, 2 m, 3 m and 5 m using 0.2 m layer thickness in every case. In addition, we tested two evenly spaced layerings, 0.1 and 0.2 m, as well as one logarithmic layer structure, in a 2 m deep peat column. The logarithmic structure was based on the one used in the land surface model JSBACH (Ekici et al., 2014) and the layer thicknesses from top to bottom were 0.06, 0.13, 0.26, 0.52 and 1.03 m.

3.32.34 Interecomparison – Comparison of HIMMELI and measured CH_4 fluxes in the Siikaneva and Lompolojänkä sites

In order to demonstrate that HIMMELI outputs realistic fluxes when run with realistic input – which is not so evident if looking only at the mechanistic sensitivity tests – we compared We compared the modelled and measured CH_4 fluxes simulated when testing the model sensitivity to peat column description with CH_4 fluxes observed at Siikaneva on two sites, Siikaneva and Lompolojänkä (Sect. 3.4) using anoxic respiration estimated for the sites as input. The purpose of this intercomparison also was a general evaluation of how well HIMMELI is able to simulate the observations and what is its the significance of using HIMMELI compared to using (simulated) anoxic respiration rate directly as the basis of CH_4 emission estimations. When comparing model and measurements, the dataset consisted only of those days from which the measured CH_4 flux was available.

3.43 Siikaneva site and measurements Peatland sites and data

3.4.1 Siikaneva site description

The eddy covariance flux measurement site is located in Siikaneva in Ruovesi, Southern Finland ($61^\circ 49' \text{ N}$, $24^\circ 11' \text{ E}$, 162 m a.s.l.) (Rinne et al., 2007). The site is a boreal oligotrophic fen where the vegetation is dominated by sedges (*C. rostrata*, *C.*

limosa, *E. vaginatum*), Rannoch-rush (*Scheuchzeria palustris*) and peat mosses (*Sphagnum balticum*, *S. majus*, *S. papillosum*). Peat depth at the measurement footprint is 2--- to 4 m. Annual mean temperature in 1971--- to 2000 at a nearby weather station was 3.3° C and precipitation 713 mm (Drebs et al., 2002). Siikaneva is a well-established site following the common standards and requirements for eddy-covariance measurements and its characteristics and representativeness of the data has been
5 analyzed in several papers (Aurela et al., 2007; Rinne et al., 2007).

~~We drove the model with daily averages of WTD, peat temperature profile, LAI and anoxic respiration rate, and compared the results with daily medians of CH₄ flux data from years 2005...2011. Simulation of LAI and anoxic respiration are described in Appendix B. Peat temperature has been monitored in Siikaneva at five depths: 5 cm, 10 cm, 20 cm, 35 cm and 50 cm. We created the temperature profile by interpolating linearly between the measurements. To obtain temperatures below the 50 cm depth we assumed that the temperature at 3 meters depth is constant at +7°C that was the mean temperature of all the years at 50 cm depth according to the measurements. Gaps in the measurement data were filled by linear interpolation. Soil temperature data from levels 10 and 40 cm was missing over a longer period so this gap was filled by linear interpolation between the adjacent measurement depths. The main component of the input anoxic respiration was derived from simulated~~
10 ~~NPP. The NPP model was driven with the WTD, photosynthetically active radiation (PAR) and air temperature (T_{air}). Long gaps in PAR and T_{air} data were filled by using corresponding data from a nearby measurement station SMEAR II (Hari and Kulmala, 2005). Simulation of LAI and anoxic respiration are described in Appendix B.~~

The measurement setup for CH₄ fluxes consisted of an acoustic anemometer and a fast response CH₄ analyzer. The acoustic
20 anemometer was Metek USA-1 during the whole measurement period, while there were changes in the methane analyzers. The CH₄ analyzers used were Campbell TGA-100 (2005--- to 2007 and 04/2010--- to 08/2010), Los Gatos RMT-200 (2008...2011) and Picarro G1301-f (04/2010--- to 10/2011). For CO₂ and water vapor fluxes a closed path infrared absorption gas analyzer LiCor 7000 was used. The sonic anemometer and the intake for the CH₄ analyzer were at 2.75 m from peat surface. The sample air taken to the TGA-100 was dried using Nafion drier. For RMT-200 and G1301-f sample air was not
25 dried. The measurement setup for 2005--- to 2007 has been described in detail by Aurela et al. (2007) and Rinne et al. (2007).

The flux data were post-processed using EddyUH software (Mammarella et al., 2016). The fluxes were calculated using block-averaging and sector-wise planar fitting. High frequency losses were corrected by empirically determined transfer functions (Mammarella et al., 2009). For 2008--- to 2011, the dilution effect by water vapor were corrected with Webb-Leuning-Pearman
30 method (Webb et al., 1980), whereas for 2005--- to 2007 this correction was not needed due to the usage of a drier in the sampling line.

3.4.2 Lompolojänkkä site description

5 The Lompolojänkkä measurement site is an open, nutrient-rich sedge fen located in the aapa mire region of north-western Finland (67°59.832'N, 24°12.551'E, 269 m above sea level). The vegetation layer is dominated by *Betula nana*, *Menyanthes trifoliata*, *Salix lapponum* and *Carex spp.* with mean vegetation height of 40 cm and one-sided leaf area index (LAI) of 1.3. The moss cover on the ground is patchy (57% coverage), consisting mainly of peat mosses (*Sphagnum angustifolium*, *S. riparium* and *S. fallax*) and some brown mosses (*Warnstorfia exannulata*). The mean annual temperature of -1.4 °C and precipitation of 484 mm have been measured at the nearest long-term weather station of Alamuonio (67°58'N, 23°41'E) during the period 1971 to 2000 (Drebs et al., 2002).

10 The eddy covariance system used for measuring the vertical CO₂ and CH₄ fluxes included a USA-1 (METEK) three-axis sonic anemometer/thermometer, a closed-path LI-7000 (Li-Cor, Inc.) CO₂/H₂O analyser and RMT-200 (Los Gatos Research) CH₄ analyzer. The measurement height was 3 m and the length of the inlet tubes for the LI-7000 and RMT-200 were 8 m and 15 m, respectively. The mouths of the inlet tubes were placed 15 cm below the sonic anemometer and flow rates of 5 to 6 l min⁻¹ and 16 l min⁻¹ were used for LI-7000 and RMT-200, respectively. Synthetic air with a zero CO₂ concentration was used as the reference gas for LI-7000. For more details of the eddy covariance measurement system, see Aurela et al. (2009).

15 Half-hour flux values were calculated using standard eddy covariance methods. The original 10-Hz data were block-averaged, and a double rotation of the coordinate system was performed (McMillen, 1988). The time lag between the anemometer and gas analyzer signals, resulting from the transport through the inlet tube, was taken into account in the on-line calculations. An air density correction related to the sensible heat flux is not necessary for the present system (Rannik et al., 1997), but the
20 corresponding correction related to the latent heat flux was made (Webb et al., 1980). Corrections for the systematic high-frequency flux loss owing to the imperfect properties and setup of the sensors (insufficient response time, sensor separation, damping of the signal in the tubing and averaging over the measurement paths) were carried out off-line using transfer functions with empirically-determined time constants (Aubinet et al., 2000). We used here a gapfilled time series, in which measurement gaps were filled with running means.

25 **3.4.3 Input data preparation**

We forced the model with daily averages of WTD, peat temperature profile, LAI and anoxic respiration rate, and compared the results with daily medians of CH₄ flux data from years 2005 to 2011 from Siikaneva and daily averages of CH₄ fluxes from years 2006 to 2010 from Lompolojänkkä. Simulations of LAI and anoxic respiration are described in Appendix B.

30 In Siikaneva, peat temperature has been monitored at five depths, -5 cm, -10 cm, -20 cm, -35 cm and -50 cm, and from Lompolojänkkä we had temperature data from -7 cm and -30 cm depths. We created the temperature profiles by interpolating linearly between the measurements. This was done also for the time step test (Sect. 3.3.2). To obtain temperatures below the deepest measurement points, we assumed that the temperature at -3 meters depth in Siikaneva is constant at +7°C that was the

mean temperature of all the years at -50 cm depth (according to the measurements), and at Lompolojänkkä the temperature at -2 m depth is constant +4 °C, the mean temperature of all the years at -30 cm. Gaps in the measurement data were filled by linear interpolation. At Siikaneva, soil temperature data from levels -10 and -40 cm was missing over a longer period so this gap was filled by linear interpolation between the adjacent measurement depths. The main component of the input anoxic respiration for Siikaneva was derived from simulated NPP. The NPP model was driven with the WTD, photosynthetically active radiation (PAR) and air temperature (T_{air}). Long gaps in PAR and T_{air} data were filled by using corresponding data from a nearby measurement station SMEAR II (Hari and Kulmala, 2005).

10 4 Results and discussion

4.1 Model sensitivity to input data

Via the tests, we wanted to verify that the model dynamics are robust, and to find out how sensitive the output CH_4 fluxes are to the input data. Table 4. summarizes the sensitivity results. In the following, we discuss the results, focusing on the most important aspects and primarily on CH_4 . It is worth noting that these are results from mechanistic sensitivity tests of HIMMELI, ~~and~~ not predictions about responses of CH_4 emissions to environmental factors in peatland ecosystems but about how HIMMELI will behave when it is used. For example, the total input anoxic respiration rate here was independent of WTD. WTD only governed the number of peat layers into which this input was distributed and thus the total anoxic respiration rate did not decrease with dropping WTD. Moreover, although soil respiration generally is known to depend on temperature, in these tests there was no dependency between temperature and anoxic respiration rate, which enabled observing the temperature effect within the processes in HIMMELI.

According to the model, the steady-state dissolved CH_4 concentrations increase when moving deeper in the peat column (Fig. 23). This results from the increasing hydrostatic pressure that controls the threshold concentration (pressure) above which gases are released as ebullition. As the solubility of CO_2 is higher than that of CH_4 , the saturated CO_2 concentrations were higher than CH_4 concentrations. In the example shown here, ebullition was driven by CO_2 . This can be seen in the concentration plots: CH_4 concentrations did not reach saturation, at their highest values but stabilized into a value in which where the sum of the partial pressures of N_2 , CO_2 and CH_4 was in balance with the combined atmospheric and hydrostatic pressures. LAI was 0 and thus the only transport route of O_2 into the soil was diffusion in water-filled peat pores, therefore, O_2 concentrations remained very low.

Contribution of different transport routes in the total CH_4 flux varied according to model input. Naturally, when LAI was 0, no CH_4 was emitted via plants. Furthermore, because ebullition occurring when the WTD was below the peat surface was

transferred to the lowest air-filled peat layer and the gases ~~continued-are then transported via~~ diffusion in dry peat or plant roots ~~after that~~ (see Sect. 3.1.7), the direct ebullition ~~fluxes~~ to the atmosphere ~~were zero~~ occurred only when WTD was below at or above the peat surface. Increasing LAI increased the relative contribution of plant transport in the total CH₄ emission in tests L_W0_T10_R1 and L_W03_T10_R1 (Fig. 34a; Table 42). Generally, the proportion of plant transport in the total CH₄ emissions correlated negatively with the total emission rate, which can be seen in particular in the test R_W0_L1_T10 where LAI was constant 1 and input respiration varied (Fig. 43b). The underlying mechanism here was that high input respiration, i.e. high CH₄ and CO₂ production, enhanced ebullition (or ebullition followed by transport via diffusion in soil layers above the WTD in cases with WTD < 0) – as could be expected.

10 Anoxic respiration rate and the corresponding potential methane production rate (PMP) (tests starting with R_) governed the outputted CH₄ emissions. The total emissions depended strongly on the PMP and were only modestly modified by LAI and WTD. The dependency between PMP and CH₄ emission was linear with R² of 1.0 in the cases that LAI was zero and greater than 0.99 in the cases with LAI of 1 m² m⁻² (Fig. 45). The percentage of PMP released as CH₄ emission varied between 245% and (almost) 100%, the smallest percentages occurring with the lowest anoxic respiration rates. Generally, the lowest values were obtained from the test R_W0_L1_T10 because this combination allowed the highest inhibiting effect by O₂ (the underlying mechanism is discussed below). The highest emissions occurred when both WTD and LAI were zero in test R_W0_L0_T10. The strong dependency between anoxic respiration and CH₄ emission was also demonstrated in the transition test (Fig. 56). The increase/decrease in input respiration affected directly the output CH₄ emission rate.

20 In the tests in which the input respiration was constant and we analyzed the sensitivity of CH₄ fluxes to LAI, WTD and temperature, the final total steady-state CH₄ emission rates varied from 468% to almost 100% of PMP. All the test results combined (Fig. 67), the most important governing factor seemed to be LAI; the high emissions required LAI being zero because that minimized the O₂ transport into the soil. Secondarily, WTD controlled the fluxes. The highest emissions occurred when, in addition to zero LAI, WTD was zero or above the peat surface. Effect of temperature was the least important of the input factors, unlike probably in models that describe the total carbon cycle where the rate of anoxic respiration depends on temperature. In our tests, temperature affected only those processes that HIMMELI itself simulates (transport, oxidation, aerobic respiration). However, also with HIMMELI the largest CH₄ emissions occurred in the tests with high temperatures.

30 Although temperature did not affect significantly in steady state, temperature change in the temperature transition tests had a clear effect on the CH₄ emissions (Fig. 8). A two-degree abrupt temperature rise throughout the peat column caused the emissions to peak momentarily, before settling to a level only moderately higher than before. The two-degree temperature drops were, correspondingly, followed by a few days clear depression in the emissions, until they gradually recovered back to the normal level. This resulted from temperature transitions changing the gas solubilities and thus the volume of gases available for ebullition.

One interesting result was that the CH₄ emissions decreased with decreasing WTD in test W_L0_T10_R1 in which plant transport played no role (Fig. 79a). This was controlled by the oxidation rate that depends on the thickness of the dry oxic peat layer. However, when plant transport was included in W_L1_T10_R1, the highest emissions occurred with the deepest WTD (Fig. 79b) because then the root mass available for transporting O₂ into the CH₄-producing peat layers was at its lowest. The same trends were obvious in the transition tests with changing WTD (Wtr_L1 and Wtr_L0; Fig 108), dropping WTD caused increasing emissions when LAI was 1 but decreased them when LAI was 0.

The main conclusion that can be deduced from the results reviewed above is that O₂ concentration was an important player in the simulations. It affected both the inhibition of CH₄ production and oxidation of CH₄ to CO₂ (Equations 6 and 8). In the tests with constant input respiration (tests ending with _R1), the actualized CH₄ production rate varied from 378% to (very close to) 100% of the PMP, and the highest inhibition of CH₄ production (i.e., lowest CH₄ production) occurred with high LAI that allowed high O₂ plant transport into the soil. The same pattern was obvious in the tests on varying input respiration (R_). When LAI was zero, the CH₄ production was more or less equal to the PMP. When LAI was 1 and WTD was -0.3 m, the production was 935% to 98% of the PMP. When LAI was 1 and WTD was 0, i.e., all the roots were inundated, the production was at its lowest and varied between 53% and 741% of PMP. This indicates that the more O₂ was transported to those soil layers that produced CH₄, the less CH₄ was produced and consequently emitted. Whether the same production was distributed either in the entire 2 m peat column or only e.g. in the bottom 1.7 m, was significant since in the latter case, there was less O₂ transported as a whole to the CH₄-producing soil layers, because the greatest root mass is allocated into the topmost peat layers.

The impact of temperature on the output fluxes in the steady-state tests was also transmitted via O₂ availability. A one-degree increase in peat temperature increased the total methane emissions on average by 0.0940 nmol m⁻² s⁻¹ (0.01 to 0.02%) without gas-transporting vegetation (T_W0_L0_R1) and 7.21.6 nmol m⁻² s⁻¹ (0.31.4%) with vegetation (T_W0_L1_R1). The dependencies were linear with R² of 0.98 and 0.991.0, respectively. The main reason for this was that in cold temperatures, the solubility of gases, and thus the concentrations of dissolved O₂ in water were higher. Therefore, the CH₄ oxidation and inhibition of CH₄ production were highest in low temperatures although the rates of these reactions were at their lowest (Eq. 9).

The tests thus revealed that O₂ transport and other O₂-related processes also deserve attention in CH₄ modelling, when O₂ concentrations are simulated. It is known that the strictly anoxic methanogens are inhibited by O₂ (Celis-García et al., 2004) and so it is important to have a proper description of the inhibition process in the CH₄ models. O₂ transport of aerenchymatous plants has been measured in laboratory conditions (Moog and Brüggemann, 1998) and in the field (Mainiero and Kazda, 2004) but there seem to be no studies in which the simulated plant transport of O₂, its dependency on model inputs like LAI or even the dissolved O₂ concentrations have been compared with measurements. Measuring O₂ fluxes with traditional chambers is

challenging because detecting small changes in the high atmospheric O₂ concentration (21%) is difficult (Brix and Sorrell, 2013). Consequently, observational O₂ data for validating the O₂ side of CH₄ models is largely lacking.

As mentioned above, effects of the input factors on CH₄ emissions may be different when taking the whole peatland carbon cycle into consideration. For example, in test L_W0_T10_R1 high LAI meant high CH₄ plant transport capacity that intuitively could mean high CH₄ emissions. However, here the impact of increased plant transport of O₂ into the soil was so strong that as a result, the total CH₄ emissions were lower with high LAI (Fig. 911). Root exudates of gas-transporting plants have been suggested to be a significant source of CH₄ substrates (Whiting and Chanton, 1993), and unlike in these sensitivity tests, a greater LAI would probably also mean higher CH₄ substrate input in nature. We tested this by setting the input respiration to depend linearly on LAI, assuming zero respiration when LAI=0. In this case, the total CH₄ emissions depended on the input respiration and increased with increasing LAI, as could be expected to happen when HIMMELI is connected to a full peatland carbon model.

Direct comparison of our results and sensitivity studies done on other peatland CH₄ emission models is not worthwhile because the other studies have analyzed the response of the total peatland carbon model. Some observations can, however, be made. In several studies the parameters affecting the CH₄ production rate have been found important (Wania et al., 2010; Berrittella and van Huissteden, 2011), which corresponds to our result that the input anoxic respiration rate affects the output significantly. Wania et al. (2010) tested the effect of tiller porosity on the CH₄ emissions and found that at four out of five of their sites, greater porosity increased the total CH₄ flux because of enhanced plant transport of CH₄, despite the fact that also O₂ transport increased. However, in their model, O₂ did not affect the CH₄ production rate. In our tests, PMP was not dependent on temperature and hence the total effect of temperature was mediated via gas solubilities and rates of oxidation and inhibition. In a complete peatland model, also CH₄ production will depend on temperature and as the temperature sensitivity of CH₄ production is known to be high (Segers, 1998), probably that would outweigh the other temperature dependencies (Riley et al., 2011). For the development of process-based CH₄ models, it is thus useful to analyze the effects of temperature also independently of carbon input. Tang et al. (2010) studied the response of their models to changes in WTD and found that increasing the WTD retarded the CH₄ emissions probably because the diffusivity in water is lower than in the air. Whether the increasing WTD affected the total CH₄ production is not discussed in their study.

4.2 Effect of diurnal temperature variation and time step length

Comparing the outputs of the model run using a 30-min time step with the outputs from the run with a daily time step showed that eliminating the diurnal temperature variation does not have any significant effect on the model output. When using the shorter time step, diurnal variation in the flux was evident and, for instance, a small (around 0.05 to 0.1 degrees) temperature increase throughout the peat column below 0.5 m depth during the last hour caused a clear peak in the emissions (Fig. 12). However, within this set-up, the daily average CH₄ emission rate of the 30-min run and the daily output from the 1-day run

were equal to two decimal places, $0.27 \mu\text{mol m}^{-2} \text{s}^{-1}$. The simulation did not relate the anoxic respiration rate to temperature, however, this result indicates that HIMMELI produces consistent output irrespective of the time step length.

4.23 Model sensitivity to the description of the peat column

The sensitivity tests with different soil layerings and peat thicknesses conducted using the input data set from Siikaneva site showed that the set-up of the peat column does not have any significant effect on the output. The mean total CH_4 flux was between 137.5 and $148.5 \text{ nmol m}^{-2} \text{s}^{-1}$ for all the set-ups. There were no striking differences in the simulated time series (Fig. 103) and so they all followed the measured CH_4 fluxes similarly (Fig. 144a). The same applied to plant transport of CH_4 ; the mean plant-transported flux was approximately $144 \text{ nmol m}^{-2} \text{s}^{-1}$ in all the cases. Direct ebullition to the atmosphere occurred only a few times during this seven-year simulation and so it was not a significant contribution to the total CH_4 emissions (thus not shown). The maximum peak direct ebullition to the atmosphere (daily average) fell between 11 to $125 \text{ nmol m}^{-2} \text{s}^{-1}$ in all other cases except with the logarithmic layering it was around $17 \text{ nmol m}^{-2} \text{s}^{-1}$. The remains of the total flux, the mean being approximately between 3 to $4 \text{ nmol m}^{-2} \text{s}^{-1}$ in each case, was transported by diffusion in the peat. This diffusion flux contained ebullited CH_4 that originated from the water-filled peat layers when the WTD was below the peat surface, which was mostly the case. Also the total CO_2 flux was similar in all the set-ups (13d). The mean total CO_2 flux was 1.1 to $1.2 \mu\text{mol m}^{-2} \text{s}^{-1}$ in all the cases.

This sensitivity test indicated that when simulating CH_4 fluxes with HIMMELI, it is not worthwhile to describe a deep peat column with dense layering because it does not significantly improve the accuracy of the simulation compared with a faster set-up, such as a logarithmic layer structure that is often used in land surface models. The logarithmic layering gave – within the experimental accuracy – the same similar result as the 10 cm layers, when the input data was the same. Principal reasons probably were that the CH_4 production was now allocated mainly to the topmost peat layers, following the vertical root distribution (Eq. 4) and that the CO_2 flux was driven by aerobic peat respiration in layers above the WTD. The emission peaks of all the different set-ups coincided in 2010, despite the fact that the peat thicknesses differed. Based on the temperature transition tests, the underlying mechanism reason here seemed to be was that concentrations in pore water at certain depths always saturated at approximately similar levels and thus a relatively abrupt temperature rise in peat layers, which did not occur in other years. This, probably together with the sinking WTD, triggered ebullition from the water-filled peat layers similarly in all the cases. The ebullited CH_4 is seen as a peak in the diffusion flux. This may, however, depend on the WTD range used.

4.34 Intercomparison-Comparison of modelled and measured CH_4 fluxes

The anoxic respiration inputs created for Siikaneva and Lompolojännkä (Appendix B) had a clear annual pattern and the rates varied between 0.02 to $0.6 \mu\text{mol m}^{-2} \text{s}^{-1}$ for Siikaneva and between 0.01 to $1.5 \mu\text{mol m}^{-2} \text{s}^{-1}$ for Lompolojännkä. This magnitude

is within literature values. Szafranek-Nakonieczna and Stepniewska (2014) observed anaerobic CO₂ production in peat incubations ranging up to around 0.1 g(CO₂) kg⁻¹ (dry weight) d⁻¹, which corresponds to around 4 μmol m⁻² s⁻¹ assuming peat bulk density of 80 g dm⁻³ (Turunen et al., 2002) and 2 m of peat. A model of peat respiration, parameterized by Riutta et al. (2007) using measurement data from a peatland site similar to Siikaneva, gave respiration rate of 0.5 μmol m⁻² s⁻¹ at air temperature of 20°C and WTD of zero (full inundation).

Figure 14 shows the daily observed CH₄ fluxes and the CH₄ fluxes simulated using the logarithmic layer structure in a 2 m deep peat column at Siikaneva and Lompolojännkä. Magnitude of the modelled emissions is comparable to the observed fluxes although there is some difference, especially at Lompolojännkä. The measured CH₄ emissions were on average 80% and 140% of the modelled emissions at Siikaneva and Lompolojännkä, respectively. It is also clear, especially at Lompolojännkä, that the simulated annual emission pattern deviates from the observations; the modelled emissions tend to increase too late in spring and decrease too early in the autumn. This may be partly due to a biased presentation of changes in LAI but principally the reason was a biased annual pattern of input anoxic respiration. The main component of the anoxic respiration was derived directly from simulated daily NPP and it produced CH₄ and CO₂ immediately, without any time lag, for example, via pools of decomposing organic compounds that could be important at least in the autumn. ~~Simulated NPP (that formed the main part of the anoxic respiration) or the LAI curve may have been biased or the way how the anoxic respiration depended on NPP may have been too straightforward. It now depended directly on the daily NPP and produced CH₄ and CO₂ immediately, there were no pools of potential CH₄ substrates. In reality, as well as in soil carbon models with which HIMMELI could be combined, there is some lag in the process of carbon fixation turning into root exudates and further to CH₄.~~ Most probably both the magnitude and the annual pattern of the emissions can be improved by more realistic simulation of anoxic respiration. However, the model explained the variation in emissions relatively well: the R² between model and measurement was 0.63 at Siikaneva and 0.70 at Lompolojännkä.

The simulated CO₂ emissions were also at realistic levels both at Siikaneva and Lompolojännkä. According to Aurela et al. (2007), the mean respiration in Siikaneva in July 2005 was 1.1 to 2.3 μmol m⁻² s⁻¹ and in our simulation, the mean CO₂ emission in July 2005 was 2.4 to 2.8 μmol m⁻² s⁻¹ (Fig. 15). At Lompolojännkä, monthly respiration of July 2006 to 2008 was around 2.5 μmol m⁻² s⁻¹ (Aurela et al., 2009) while the model simulated a CO₂ flux of 3.5 μmol m⁻² s⁻¹ (data not shown). The model overestimated slightly the emissions, especially given that it does not include CO₂ from autotrophic respiration unlike the observed fluxes, but the result is still reasonable.

Summer 2010 at Siikaneva was interesting since both model and measurements show the highest emission peaks then. The maximum emissions do not coincide exactly on the same days, but they are temporally close. In HIMMELI, the main reason was an exceptionally abrupt temperature rise in the peat water, followed by decreasing gas solubilities and increased ebullition

– as was observed in the temperature transition tests. Summer 2010 was unusually hot in Finland and so the heat can very well be the cause of the observed high emissions also in nature. We do not know whether the effect really can be transmitted via gas solubilities instead of, for instance, increased respiration. Grant and Roulet (2002) compared simulated and measured CH₄ emissions at a beaver pond. Their model captured some bubbling events, driven by warming soil that affected both fermentation and methanogenesis rates and gas solubilities. In our case, the simulated input anoxic respiration did not increase noticeably during this high-emission period, but our simulation may underestimate the effect of temperature. Moreover, although the soil temperature profile used to run the model was derived from measurements, it was an approximation as it was created by linear interpolation between measurement points. The temperature change of the lower peat layers may be exaggerated compared with reality. However, the modelled CH₄ emission peaks nicely matched with observations. The model followed the measurements reasonably but it underestimated the observed CH₄ emissions on average by approximately 20%. The main reason for this discrepancy was that the anoxic respiration rate calculation (App. B) deviated from that of Susiluoto et al. (2017) and we did not optimize the parameters of HIMMELI specifically for the set-up of this study but used their parameter values as such. Simulation-based input data may also have caused the divergence between the model and measurements in the autumns when generally the modelled CH₄ emissions seemed to decline too early. Simulated NPP (that formed the main part of the anoxic respiration) or the LAI curve may have been biased or the way how the anoxic respiration depended on NPP may have been too straightforward. It now depended directly on the daily NPP and produced CH₄ and CO₂ immediately, there were no pools of potential CH₄ substrates. In reality, as well as in soil carbon models with which HIMMELI could be combined, there is some lag in the process of carbon fixation turning into root exudates and further to CH₄.

Taking a closer look at the correlation between model and measurement (Fig. 11b) was relatively good and linear with low emissions but the scatter increased with emissions above 0.05 μmol m⁻² s⁻¹. The high simulated emissions were largely driven with ebullition—that in most cases was emitted as diffusion of ebullited CH₄ from the air-filled peat layer—in summertime. Flook at Siikaneva only, the model was a slightly better predictor for the measured CH₄ emissions than the anoxic respiration as such (Fig. 15 11e), with R² 0.653 vs. 0.60. Hence, considering the anoxic respiration simulation combined with HIMMELI as one unified CH₄ model, HIMMELI slightly improved the fit compared with the anoxic respiration part alone. This shows that HIMMELI is capable of simulating realistic CH₄ fluxes.

In the data set shown in the correlation plots (Fig. 15), which was limited to those days from which the measured CH₄ fluxes were available, the R² between input anoxic respiration and modelled CH₄ emissions was 0.695. In the complete simulated time series, this R² was 0.679 and when correlating the CH₄ emissions with anoxic respiration of the previous day, R² still slightly increased, up to 0.8071. In the complete time series, the simulated CH₄ emissions were on average 145% of the input anoxic respiration or 5630% of PMP. These results support the findings from the sensitivity tests (Section 4.1) that anoxic respiration rate and the corresponding PMP do govern the output CH₄ emissions, but indicate also that oxidation and inhibition

played a role in the site simulation of Siikaneva. The temperature responses of anoxic respiration and modelled CH₄ emissions were very similar (Fig. 15).

Anoxic respiration alone thus seems a good basis to estimate CH₄ emissions but a complete model of CH₄ processes is necessary, also in situations when the focus is not on studying concentration profiles or the processes in detail. Simple parameterizations have been tested against process-based CH₄ models. For example, Van Huissteden et al. (2009) compared the peatland model PEATLAND-VU that utilizes the Walter-Heimann CH₄ scheme, with an emission factor that was based on averages of measurement data on six arctic and temperate wetlands. They found that the model produced a significantly better estimate only on 50% of the sites; on the others, the simple emission factor did better or almost equally well. They concluded, however, that process models are needed for large-scale modelling. Berrittella and van Huissteden (2009) compared PEATLAND-VU to a fixed fraction of NPP as the estimate of CH₄ emissions when simulating northern wetlands in glacial climates. In this case, they naturally did not have real-time observational flux data to compare their results with, but they concluded that the two approaches gave *different* results, for instance, the simplistic NPP model produced smaller differences between glacial climates than PEATLAND-VU. A CH₄ model like HIMMELI is a significant addition to peatland carbon models, in order to be able to take into account more factors affecting CH₄ emissions.

5 Conclusions

The new model for simulating CH₄ build-up and emissions in peatlands, HIMMELI, is a robust tool to be used as the CH₄ emission model in different peatland carbon models. It runs well with different peat column set-ups and within a wide range of inputs. The simulated CH₄ emissions are not sensitive to the description of the peat column in case it does not affect the input variables. HIMMELI was able to simulate realistic CH₄ fluxes ~~observed at~~ the Finnish peatland sites Siikaneva peatland measurement site in southern Finland and Lompolojänkkä when run with measured and simulated input from the sites.

Sensitivity tests conducted on HIMMELI revealed mechanisms controlling the simulated CH₄ emissions that may remain hidden when testing the sensitivity of a full peatland carbon cycle model. Simulated CH₄ fluxes largely depended on the input anoxic respiration rate and the corresponding CH₄ production rate. This shows that in addition to correct descriptions of CH₄ and O₂ transport and oxidation processes, it is essential that the underlying CH₄ substrate production rates are realistic, in order to produce realistic CH₄ emission estimates for different purposes. Other input variables, in particular LAI and WTD, also had an impact on the CH₄ emissions in the steady-state tests. With constant input anoxic respiration (which means constant potential CH₄ production rate), the total CH₄ emission varied from +6-5 % to almost 100 % of the potential CH₄ production, depending on the combination of LAI and WTD. The results indicated that the main factor governing this was the availability of O₂ in the peat since its concentration affected the inhibition of CH₄ production as well as rates of CH₄ oxidation to CO₂.

6 Code and data availability

The FORTRAN codes of the HIMMELI model are available as a supplement of this article. The data used in these analyses are available upon request.

Appendix A

- 5 The solubilities of gases are computed following Sander (2015). The temperature (T) dependence of Henry's law constants for the three simulated compounds CH₄, CO₂ and O₂ (H_X ; M atm⁻¹) thus are (Eq. A1-A3):

$$H_{CH_4}(T) = 1.3 \times 10^{-3} \exp \left[1700 \left(\frac{1}{T} - \frac{1}{T^\theta} \right) \right] \quad (A1)$$

$$H_{O_2}(T) = 1.3 \times 10^{-3} \exp \left[1500 \left(\frac{1}{T} - \frac{1}{T^\theta} \right) \right] \quad (A2)$$

$$H_{CO_2}(T) = 3.4 \times 10^{-2} \exp \left[2400 \left(\frac{1}{T} - \frac{1}{T^\theta} \right) \right], \quad (A3)$$

- 10 where T^θ is the reference temperature, 298 K. Temperature dependent diffusivities of the three compounds in water ($D_{X,w}$; m² s⁻¹) and in air ($D_{X,a}$; m² s⁻¹) are calculated following Tang et al. (2010) (Eq. A4-A9). The reference temperature $T^{\theta b}$ used in Equations A7-A9 is 273.15 K.

$$D_{CH_4,w}(T) = 1.5 \times 10^{-9} \frac{T}{T^\theta} \quad (A4)$$

$$D_{O_2,w}(T) = 2.4 \times 10^{-9} \frac{T}{T^\theta} \quad (A5)$$

15 $D_{CO_2,w}(T) = 1.81 \times 10^{-6} \exp \left(\frac{-2032.6}{T} \right) \quad (A6)$

$$D_{CH_4,a}(T) = 1.9 \times 10^{-5} \left(\frac{T}{T^{\theta b}} \right)^{1.82} \quad (A7)$$

$$D_{O_2,a}(T) = 1.8 \times 10^{-5} \left(\frac{T}{T^{\theta b}} \right)^{1.82} \quad (A8)$$

$$D_{CO_2,a}(T) = 1.47 \times 10^{-5} \left(\frac{T}{T^{\theta b}} \right)^{1.792}. \quad (A9)$$

Appendix B

- 20 LAI is not continuously monitored at [the peatland sites Siikaneva and Lompolojänkä](#), therefore, we utilized the method introduced by Wilson et al. (2007) to obtain LAI input data for the ~~Siikaneva~~ model runs. We simulated the LAI with a lognormal function (Wilson et al., 2007) (Eq. B1):

$$LAI(j) = LAI_{max} \times e^{\left(-0.5 \left(\frac{\ln\left(\frac{j}{j_{max}}\right)}{s}\right)^2\right)} \quad (B1)$$

where LAI_{max} is the peak LAI of the growing season, j is the Julian date, j_{max} is the Julian date when the LAI peaks, and s denotes the shape of the curve. Values for the parameters j_{max} and s (Table B1) for Siikaneva were derived from Wilson et al. (2007) by averaging the values reported for the species abundant at Siikaneva, but for Lompolojänkkä we used different j_{max} as LAI can be expected to peak earlier at the northern latitudes (Raivonen et al., 2015). The growing season peak LAI in the eddy covariance footprint area at Siikaneva was approximately $0.4 \text{ m}^2 \text{ m}^{-2}$ (Riutta et al., 2007) and $1.3 \text{ m}^2 \text{ m}^{-2}$ at Lompolojänkkä (Aurela et al., 2009). We also chose to add a constant wintertime LAI in the model since it is known that a significant green sedge biomass, approximately 15% of the maximum, may overwinter (Bernard and Hankinson, 1979; Saarinen, 1998). The maximum being $0.4 \text{ m}^2 \text{ m}^{-2}$, this meant overwintering LAI would thus be of up to $0.05 \text{ m}^2 \text{ m}^{-2}$ for Siikaneva and 0.195 for Lompolojänkkä. We used the same LAI for all the years.

The input ~~input~~ anoxic respiration was created from two components: simulated net primary production (NPP) and temperature-dependent anoxic peat decomposition V_{pR} ($\text{mol m}^{-2} \text{ s}^{-1}$). As methanogens seem to be keen on fresh, newly fixed carbon (Couwenberg & Fritz 2012), such as the root exudates, many models relate the CH_4 production rate directly with the NPP of the wetland vegetation (Wania et al. 2010, Walter & Heimann 2000, Zhuang et al. 2004) was estimated following closely the parallel study Susiluoto et al. (2017) in which the HIMMELI parameters were optimized for Siikaneva. We simply simulated the NPP time series for the sites, allocated the NPP vertically along the root distribution (Eq. 4), and removed the fraction that was in aerobic conditions, i.e., above the WTD (based on the measured WTD time series). Susiluoto et al. (2017) simulated production of CH_4 substrates as temperature dependent anoxic peat decomposition V_{pR} ($\text{mol m}^{-2} \text{ s}^{-1}$) and decomposition of root exudates in the inundated peat layers. This was computed with a simple respiration model combined with HIMMELI. Since in the present study the focus was on testing the HIMMELI model as such, we did not involve the complete respiration model here but produced input for HIMMELI using the same components as Susiluoto et al. (2017) in a simplified form. The input respiration in our study was simply the sum of anoxic peat decomposition rate and estimated root exudate production V_{extR} ($\text{mol m}^{-2} \text{ s}^{-1}$) in the inundated peat layers, we did not simulate the actual decomposition of the root exudate pool. The soil profile for which the respiration is was computed was 2 m of peat with 0.1 m layers. This NPP was scaled so that the output visually fitted the measured CH_4 fluxes at Siikaneva using a scaling factor f_s of 0.4.

V_{extR} was estimated by taking a fixed fraction f_{extR} of the net primary productivity (NPP) of vascular vegetation, i.e., simulated net photosynthesis rate P_n ($\text{mol m}^{-2} \text{ s}^{-1}$) of vascular plants. f_{extR} (Table B1) was obtained from Susiluoto et al. (2017) and the NPP of Siikaneva was calculated by running models of gross photosynthesis (P_g) and autotrophic respiration (R) for Siikaneva. We used the P_g model for a sedge and dwarf shrub canopy by Riutta et al. (2007) (Eq. B2):

$$P_g = P_{max} \frac{I}{h+I} [1 - e^{-a \times LAI}] \times e^{-0.5 \left(\frac{T_{air} - T_{opt}}{T_{tol}} \right)^2} \times e^{-0.5 \left(\frac{d_W - d_{W,opt}}{d_{W,tol}} \right)^2} \quad (\text{B2})$$

where P_g is the CO₂ uptake rate of the canopy (mol CO₂ s⁻¹ m² ground surface area), P_{max} is the maximum potential CO₂ uptake rate (mol CO₂ s⁻¹ m² ground surface area), I (μmol m⁻² s⁻¹) is PAR, h (μmol m⁻² s⁻¹) is PAR at which half of maximum photosynthesis is reached, a is the initial slope of saturating leaf-area response function, LAI is leaf area index (Eq. B1), T_{air} (°C) is air temperature, T_{opt} (°C) is the optimal air temperature for photosynthesis, T_{tol} (°C) is temperature tolerance, d_W (cm) is WTD, $d_{W,opt}$ (cm) is the optimal WTD for photosynthesis, and $d_{W,tol}$ (cm) is WTD tolerance. The parameter values are listed in Table B1. R (mol CO₂ s⁻¹ m²) was simulated with a model parameterized for sedges only (Raivonen et al., 2015) (Eq. B3):

$$R = R_{ref} \times LAI \times e^{b \left(\frac{1}{T_{ref} - T_0} - \frac{1}{T_{air} - T_0} \right)} \times e^{-0.5 \left(\frac{d_W - d_{W,opt}}{d_{W,tol}} \right)^2}, \quad (\text{B3})$$

where R is the CO₂ release rate of the canopy, R_{ref} (mol CO₂ s⁻¹ m² leaf area) is the CO₂ release rate per unit of leaf area under reference conditions, b (K) is an exponential parameter depicting the temperature sensitivity of respiration, T_{ref} (K) is the reference temperature, and T_0 (K) is the temperature at which respiration reaches zero (Table B1).

The daily averages of net photosynthesis P_n (mol CO₂ s⁻¹ m⁻²) were calculated as the difference between P_g and R . Photosynthetically active seasons were determined by searching for dates of snowmelt in spring or arrival of snow cover in autumn from the reflected PAR data or, in some cases, using air temperature (permanently > 5°C) as the criterion. No direct measurements of P_n or vascular NPP exist for validation but the simulated P_n of year 2005 was compared with an NPP estimate derived from eddy covariance CO₂ fluxes measured that year on Siikaneva. Briefly, the estimated contributions of *Sphagnum* mosses (30%; Riutta et al., 2007) and autotrophic respiration (50%; Gifford, 1994) were subtracted from the eddy-covariance based gross primary productivity (GPP) (Aurela et al., 2007; data obtained via personal communication), and the remains were taken as an estimate of the NPP of vascular vegetation. The two NPP estimates were well correlated (with R^2 of 0.9) but the eddy-covariance based NPP was on average 1.56-fold compared with the simulated P_n . Since the latter also was lowish compared with what has been reported for similar peatlands, the final estimate of NPP for years 2005–2011 was produced by scaling the simulated P_n upwards by 1.56.

25 For Lompolojännkä, the GPP time series over years 2006 to 2010 was available (Aurela et al., 2009), thus, we derived the NPP of vascular vegetation directly from the GPP data. Again we assumed that autotrophic respiration contributes 50% to the GPP (Gifford, 1994) and the contribution of *Sphagnum* was estimated to be 10%, based on the biomass values reported for Siikaneva and Lompolojännkä (Li et al., 2016).

30 The anoxic peat respiration for both sites was computed for the peat layers below WTD using the Q₁₀ model for catotelm decomposition presented in Schuldt et al. (2013) (Eq. B4):

$$V_{pR} = \sum_{z_{min}}^{WTD} Q_{10} \frac{T(z)-T_{ref,pR}}{10} \frac{1}{\tau_c} \rho_C dz. \quad (B4)$$

Here Q_{10} is the base for temperature dependence of respiration, $T_{ref,pR}$ is reference temperature for peat respiration (K), τ_{cato} is turnover time of the catotelm carbon pool (s) and ρ_C (mol (C) m⁻³) is the density of the carbon pool. The parameter ~~set optimized by Susiluoto et al. (2017) included Q_{10} and τ_c , the other~~ values were taken from Schuldt et al. (2013) except for the Q_{10} we used a higher value 3.5 that was the average Q_{10} found by Szafranek-Nakonieczna and Stepniewska (2014) (Table B1).

[Supplement link]

Author contribution: S. Smolander and L. Backman developed the model. M. Raivonen participated in model development and designed and carried out the tests with contribution from L. Backman, J. Susiluoto, T. Aalto, T. Markkanen, J. Mäkelä and T. Vesala. ~~S. Smolander and L. Backman developed the model.~~ M. Tomasic, X. Li, M. Heimann, S. Sevanto, T. Kleinen and V. Brovkin contributed to the model development. J. Rinne, O. Peltola ~~and~~ M. Aurela and A. Lohila provided observational data from the Siikaneva and Lompolojänkki sites. T. Larmola, S. Juutinen and E.-S. Tuittila provided knowledge and advice about peatland methane processes for model development. M. Raivonen prepared the manuscript with contributions from all co-authors.

15 Competing interests

The authors declare that they have no conflict of interest.

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Table 1: Model parameters and their values. The reference is given in cases where the value is directly from one study, otherwise the parameter value is discussed in Section 3.2. We used for several parameters values that were obtained in a parallel study by Susiluoto et al. (2017, in prep.) in which HIMMELI was optimized for the Siikaneva measurement site.

Symbol	Definition	Value	Reference
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λ	decay length (in root distribution)	0.25174	Susiluoto–Wania et al. (2017)
f_m	fraction of anaerobic respiration becoming methane	0.5/0.25*	–/Susiluoto et al. (2017)
V_R	potential rate of aerobic respiration at 10°C [mol m ⁻³ s ⁻¹]	8.71x10 ⁻⁵	Susiluoto et al. (2017)
K_R	Michaelis constant for aerobic respiration reaction [mol m ⁻³]	0.022	Arah and Stephen (1998)
V_O	potential oxidation rate at 10°C [mol m ⁻³ s ⁻¹]	2.71x10 ⁻⁵⁴	Susiluoto et al. (2017)
K_{O_2}	Michaelis constant for O ₂ in oxidation [mol m ⁻³]	0.033	Arah and Stephen (1998)
K_{CH_4}	Michaelis constant for CH ₄ in oxidation [mol m ⁻³]	0.4034	Arah and Stephen (1998)
ΔE_R	activation energy of aerobic respiration [J mol ⁻¹]	5093000	Stephen et al. (1998)Susiluoto et al. (2017)
ΔE_O	activation energy of oxidation [J mol ⁻¹]	5049000	Susiluoto et al. (2017)
T_ϕ	reference temperature for oxidation and aerobic respiration [K]	283	Arah and Stephen (1998)
k	time constant of ebullition [s ⁻¹]	1/1800	This study
a_{mA}	root ending area per root dry biomass [m ² kg ⁻¹]	0.47085	Stephen et al. (1998)Susiluoto et al. (2017)
τ	root tortuosity	1.50	Stephen et al. (1998)Susiluoto et al. (2017)
SLA	specific leaf area of gas-transporting plants [m ² kg]	2315	Vile et al. (2005)
$f_{D,w}$	reduction factor for diffusion in water-filled peat	0.890	Susiluoto et al. (2017)
$f_{D,a}$	reduction factor for diffusion in air-filled peat	0.837	Susiluoto et al. (2017)
η	sensitivity of methanogenesis to oxygen [m ³ mol ⁻¹]	400	Arah and Stephen (1998)
σ	peat porosity	0.85	Susiluoto et al. (2017)

*The former value (0.5) was used in the steady state tests and the latter (0.25) in the model runs on Siikanen.

5 **Table 2: Summary of the steady-state sensitivity tests in which response of HIMMELI to different input combinations was analyzed.**

Test name	T (°C)	WTD (m)	LAI (m ² m ⁻²)	Anoxic respiration (μmol m ⁻² s ⁻¹)
T_W0_L0_R1	0 , 5, 10, 20, 25	0	0	1
T_W0_L1_R1	0 , 5, 10, 20, 25	0	1	1
L_W0_T10_R1	10	0	0, 0.5, 1, 2, 3	1
L_W03_T10_R1	10	-0.3	0, 0.5, 1, 2, 3	1
W_L0_T10_R1	10	-0.5, -0.3, -0.2, -0.1, 0, 0.05	0	1
W_L1_T10_R1	10	-0.5, -0.3, -0.2, -0.1, 0, 0.05	1	1
R_W0_L0_T10	10	0	0	0.01, 0.1, 0.5, 1, 5, 10
R_W0_L1_T10	10	0	1	0.01, 0.1, 0.5, 1, 5, 10
R_W03_L0_T10	10	-0.3	0	0.01, 0.1, 0.5, 1, 5, 10
R_W03_L1_T10	10	-0.3	1	0.01, 0.1, 0.5, 1, 5, 10

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5 **Table 3: Summary of the transition tests on model sensitivity to input data and the input combinations used in the tests.**

Test name	T (°C)	WTD (m)	LAI (m ² m ⁻²)	Anoxic respiration (μmol m ⁻² s ⁻¹)
Wtr_L1	10	0, -0.2, -0.4, -0.2, 0	1	1
Wtr_L0	10	0, -0.2, -0.4, -0.2, 0	0	1
Rtr_W0_L1	10	0	1	+0.5, -31, 62, 31, +0.5
Rtr_W0_L0	10	0	0	0.5, 31, 62, 31, +0.5
<u>Ttr_W0_L1</u>	<u>10, 12, 14, 12, 10</u>	<u>0</u>	<u>1</u>	<u>1</u>
<u>Ttr_W0_L0</u>	<u>10, 12, 14, 12, 10</u>	<u>0</u>	<u>0</u>	<u>1</u>

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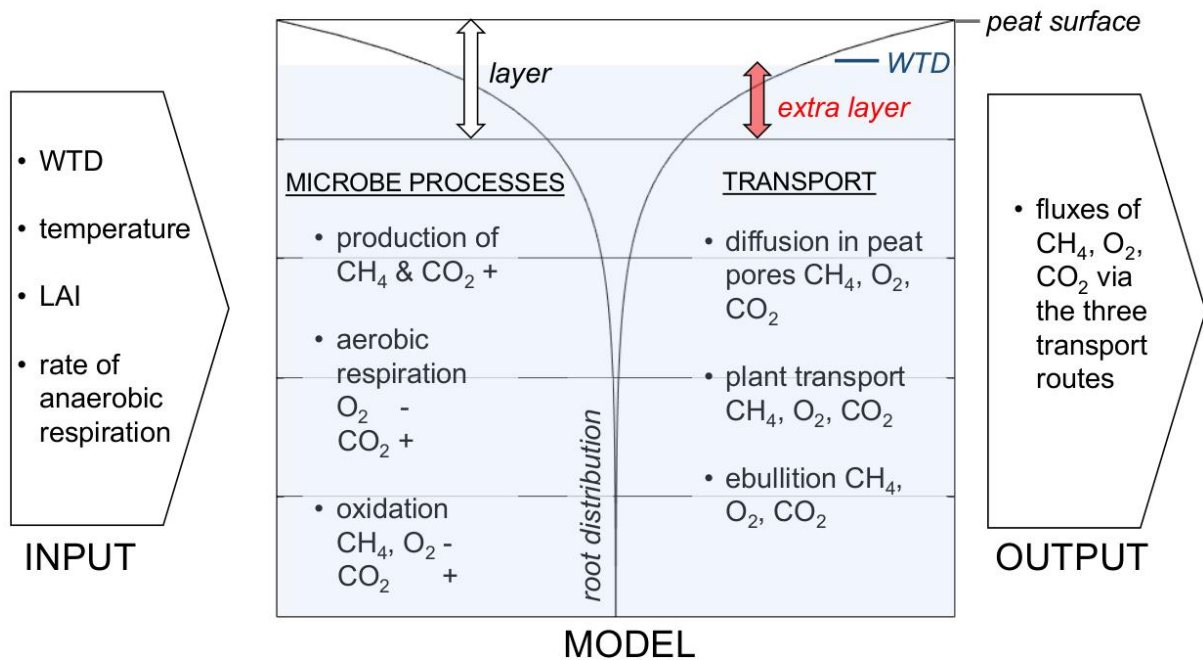
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Table 4: Results of the sensitivity testing. The rightmost column tells how much the CH₄ emissions changed when the input changed. The +/- signs in front of 'Input change' and 'Change in CH₄ emission' show the directions of change in input and the corresponding response in CH₄ emissions. This is expressed as % of **potential-CH₄-productionPMP (see Sect. 3.1.3) for the first 6 tests and as % of change in input anoxic respiration for the tests on changing input respiration. In **some-tests most cases**, the response was not constant over the input range. **In that case and therefore**, the result is also expressed as a range.**

Test	Changing input variable	Input change	Change in CH ₄ emission, % of potential production/ % of change in respiration	
T_W0_L0_R1	temperature	+1°	+ 0.02 <u>0.01</u> %... 0.02 %	
T_W0_L1_R1	temperature	+1°	+ 1.40 <u>0.3</u> %	
L_W0_T10_R1	LAI	+0.1 m ²	- 0.13 <u>0.4</u> %... 11 <u>0.3</u> %	
L_W03_T10_R1	LAI	+0.1 m ²	- 1.28 %... 1.4 %	
W_L0_T10_R1	WTD	-0.05 m	- 0.02 <u>1.4</u> %... 0.2 %	20
W_L1_T10_R1	WTD	-0.05 m	+ 0.5 <u>0.02</u> %... 10 <u>2</u> %	
R_W0_L0_T10	respiration	+	+ 98 <u>9</u> %...100%	
R_W0_L1_T10	respiration	+	+ 72 <u>2</u> %... 80 <u>7</u> %	
R_W03_L0_T10	respiration	+	+ 88 <u>9</u> %... 93 <u>7</u> %	
R_W03_L1_T10	respiration	+	+ 43 <u>2</u> %... 96 <u>2</u> %	25

Table B1: Parameter values of the models used for producing input for the Siikaneva and Lompolojänkkä runs. The value marked with * is the only one specific for the Lompolojänkkä site. The parameter V values marked with ** is fitted in this study and the value * asterisk (*) base on the study Susiluoto et al. (2017) is based on Szafrank-Nakonieczna and Stepniewska (2014), the others are from the original references of the photosynthesis and respiration models.**

Symbol	Definition	Value
P_{max}	maximum potential CO ₂ uptake [mol (C) s ⁻¹ m ⁻² ground area]	1.24x10 ⁻⁵
k	PAR at which half of maximum photosynthesis is reached [μmol m ⁻² s ⁻¹]	223.9
a	initial slope of saturating leaf-area response function	0.778
T_{opt}	optimal air temperature [°C]	24.88
T_{tol}	temperature tolerance [°C]	14.69
$d_{w,opt}$	optimal water table depth [cm]	-29.1
$d_{w,tol}$	water table depth tolerance [cm]	67.27
R_{ref}	respiration rate in reference conditions [mol (C) s ⁻¹ m ⁻² leaf area]	6.94x10 ⁻⁷
b	activation energy/gas constant [K]	300
T_{ref}	reference temperature of autotrophic respiration [K]	283.15
T_0	T at which R = 0 [K]	227.13
LAI_{max}	peak LAI	0.4
LAI_{min}	overwintering LAI	0.05
j_{max}	Julian date of the peak LAI	209/ <u>190*</u>
c	parameter to adjust the LAI curve shape	0.2
f_s	<u>NPP scaling factor</u>	<u>0.4**</u>
f_{ext}	<u>fraction of NPP converted to root exudates</u>	<u>0.4*</u>
$R_{ref,pR}$	reference temperature of peat respiration [K]	273.15
Q_{10}	base value for temperature dependence of peat respiration	<u>4.6*</u> <u>3.5***</u>
τ_C	turnover time of the catotelm carbon pool [y]	<u>1470030 000*</u>
ρ_C	density of the carbon pool [mol (C) m ⁻³]	<u>39406277.73</u>



10 **Figure 1. HIMMELI as a simplified schematic picture. The microbial and transport processes are simulated in a vertically layered one-dimensional peat column in which roots of aerenchymatous gas-transporting plants are distributed according to the exponential root distribution function. The input anoxic respiration is distributed along the root distribution. Input water table depth (WTD) determines the thickness of the possible extra layer that is introduced in case the WTD does not match any of the fixed background layer borders. This ensures that all the simulated layers are either completely water-filled or air-filled. The + sign shows that the compound is produced in the microbial process and – sign means consumption of the compound.**



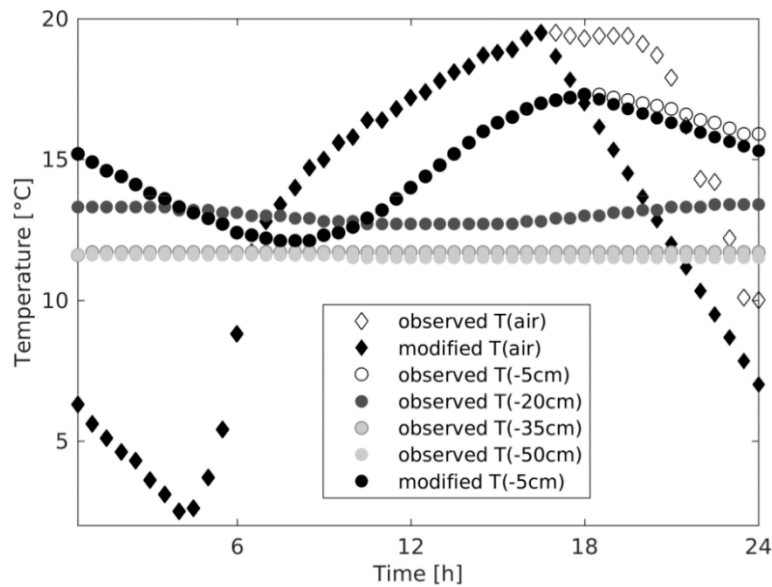
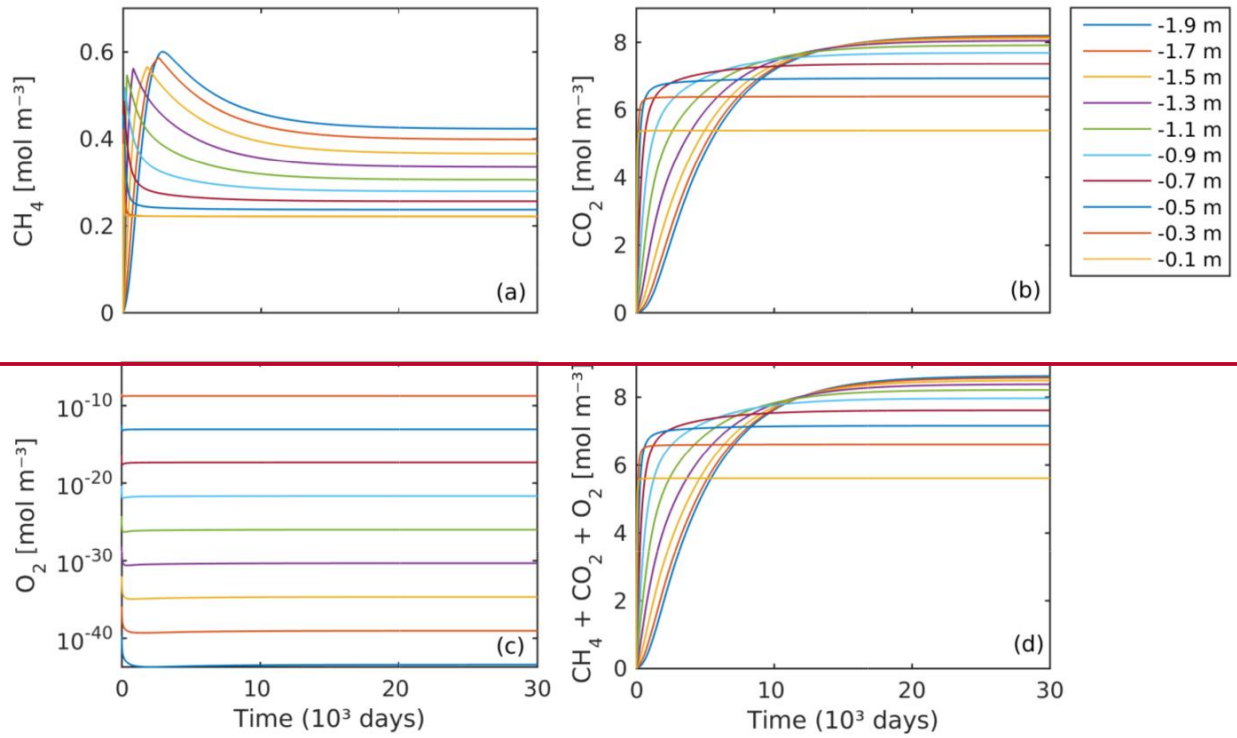


Figure 2. Daily variation of air and soil temperatures in the time step test. Observed temperatures are directly from measurement data but in order to smooth the difference between the last and first temperatures of the day, we modified the afternoon temperatures as shown in the plot.

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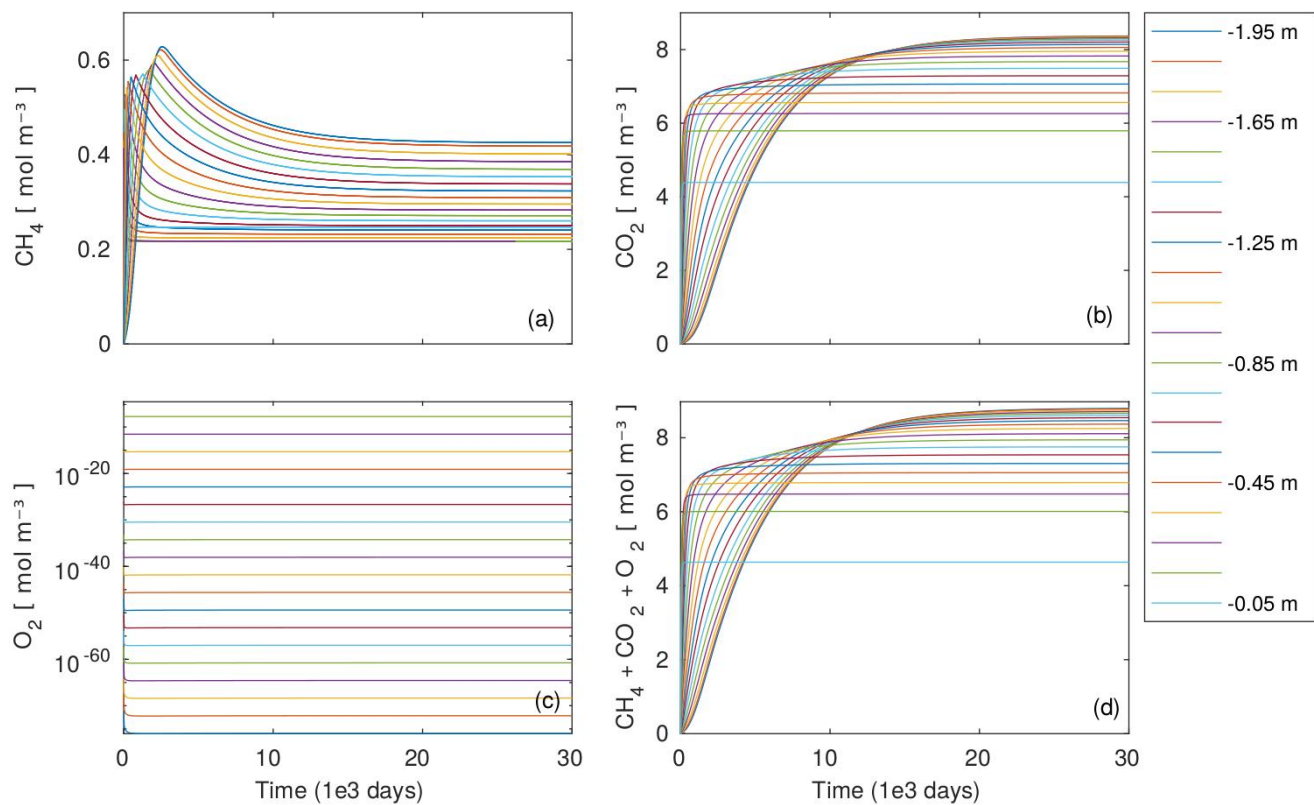
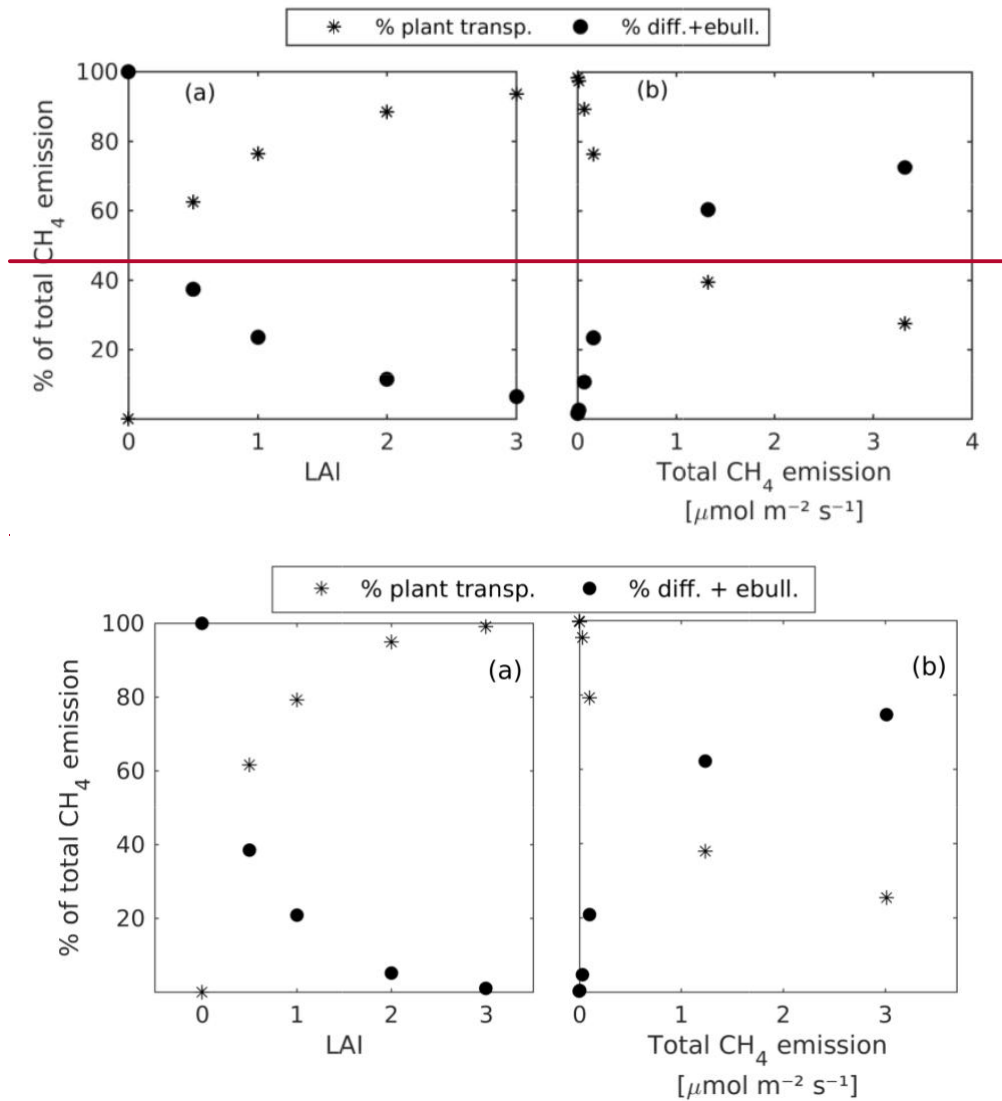


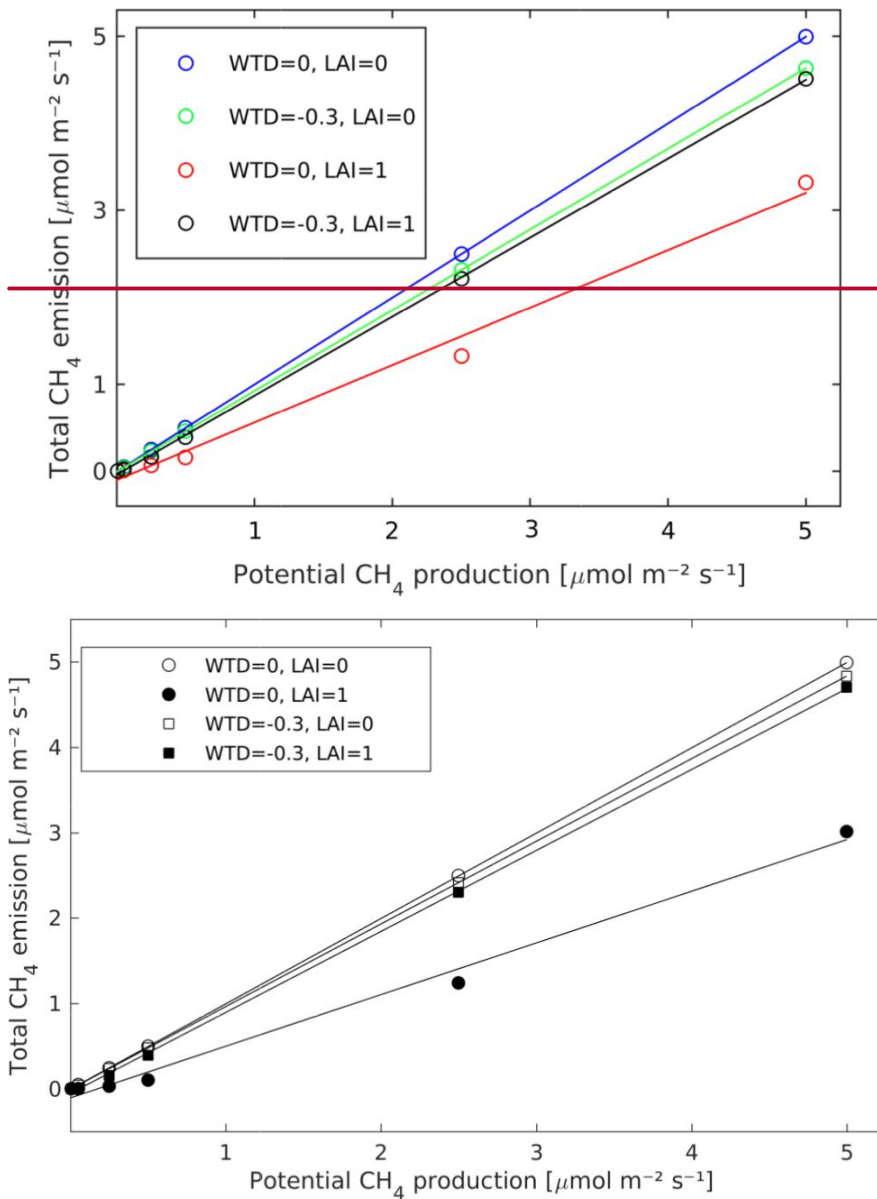
Figure 23. Evolution of the concentration profiles of (a) CH_4 , (b) CO_2 (c) O_2 and (d) their sum in a simulation where both WTD and LAI were zero, i.e., there was no plant transport of these compounds. Different colors show the concentrations at different depths in the peat. In the beginning of the simulation, all the concentrations were zero.

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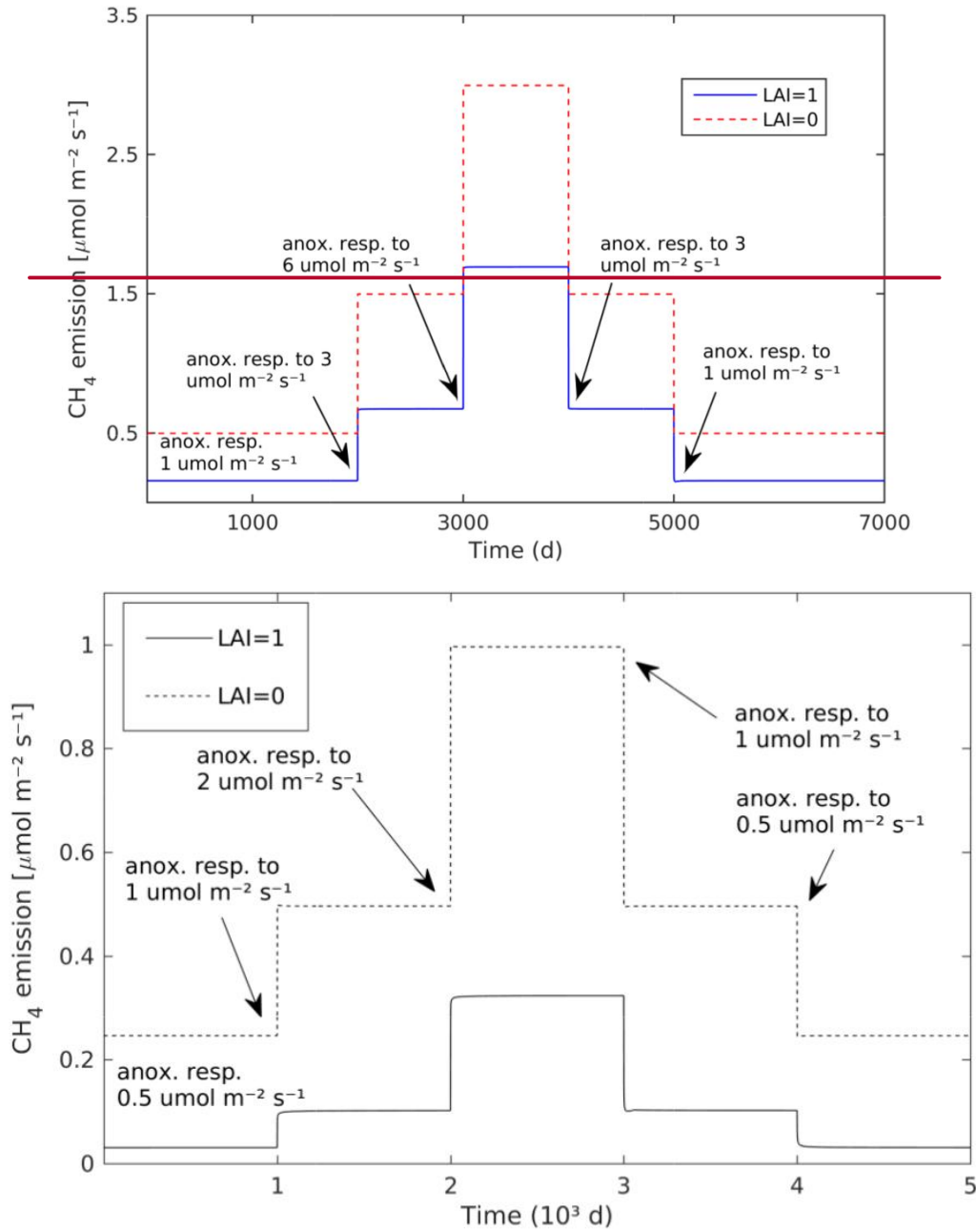
5 **Figure 34.** Contribution of different transport routes to the total CH₄ emission (a) as a function of LAI in test L_W0_T10_R1 and (b) as a function of total CH₄ emission in test R_W0_L1_T10.



5 **Figure 45.** Dependence of the total output CH₄ emission on the potential CH₄ production rate in tests on the model sensitivity to input anoxic respiration, i.e. tests that were named starting with R_.

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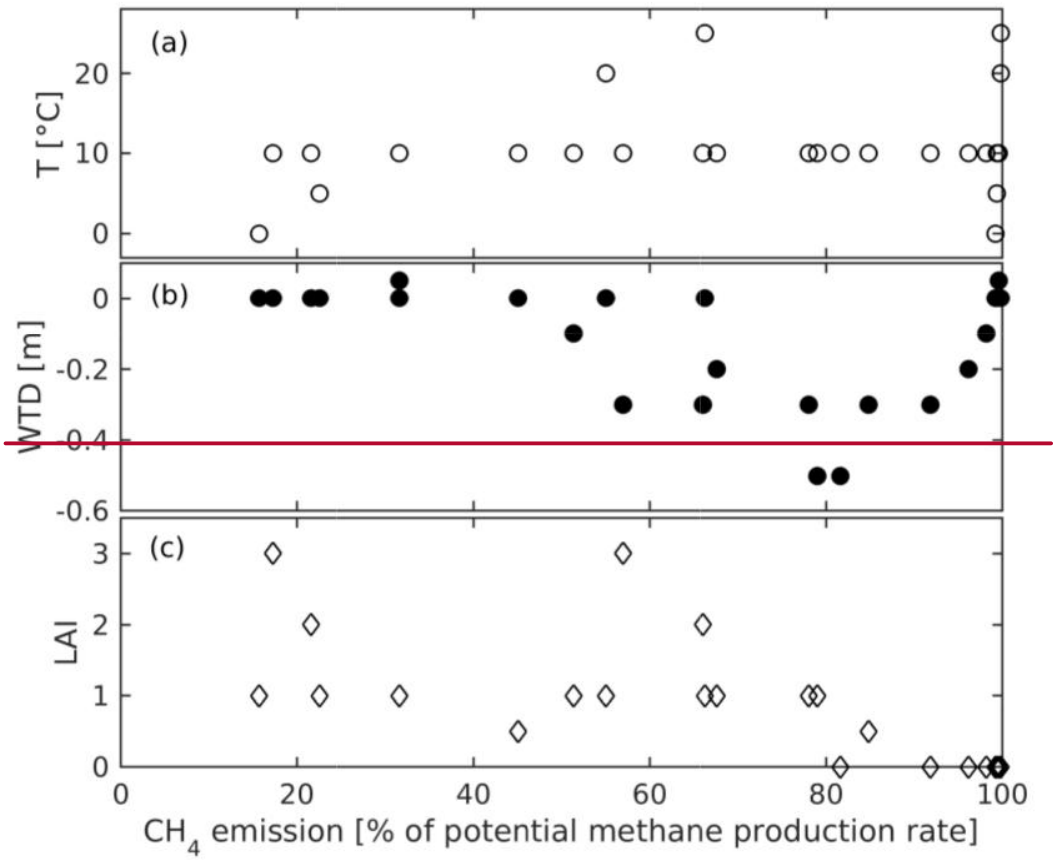
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5 **Figure 56.** Output CH₄ emission responded clearly to changes in the input anoxic respiration rate in the transition tests Rtr_W0_L1 (blue-solid line) and Rtr_W0_L0 (red-dashed line) (see Table 3). Black arrows indicate when the input changed.

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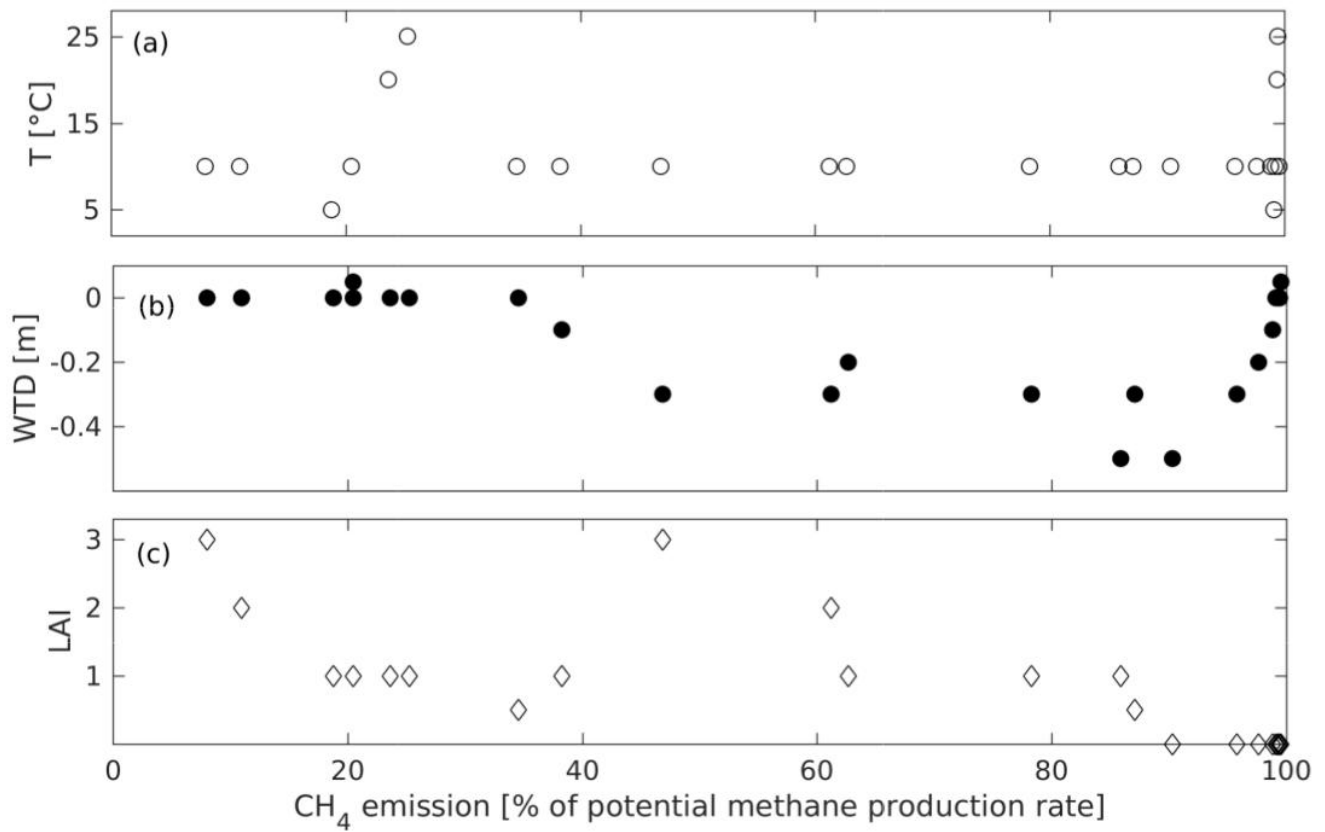
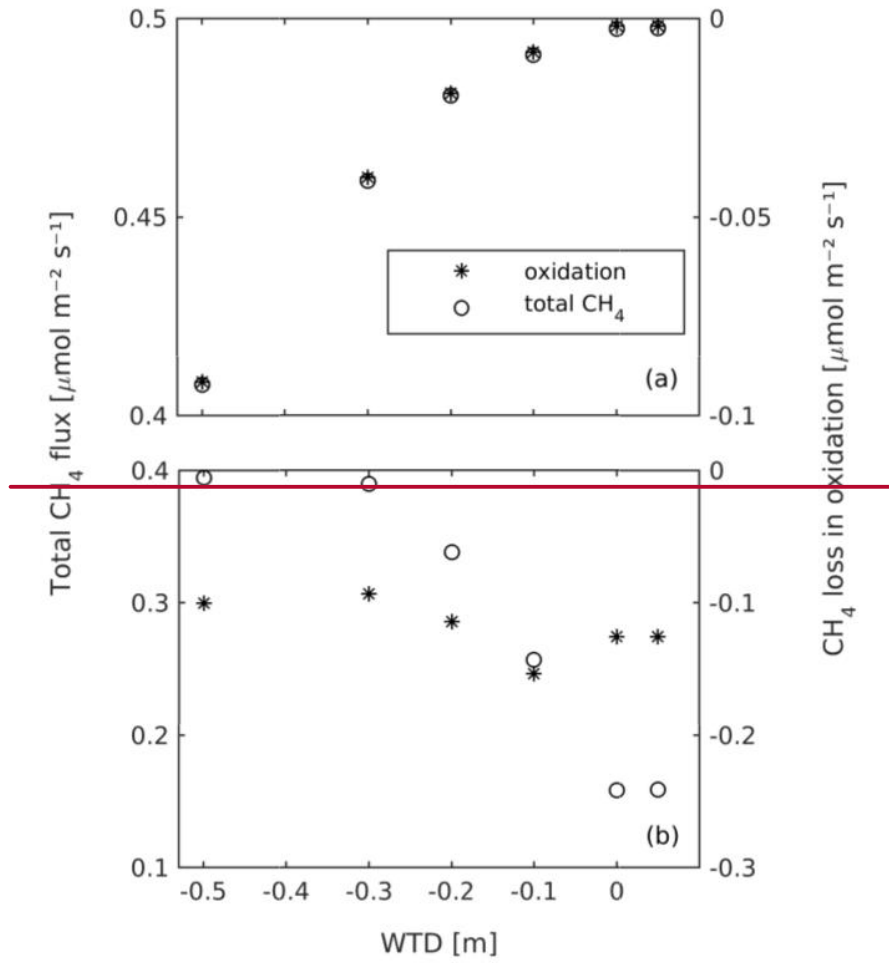


Figure 76. Relationship between the relative CH₄ emission rate (expressed as % of **potential-CH₄-productionPMP**) and different combinations of input (a) temperature, (b) WTD and (c) LAI in the steady-state sensitivity tests with constant anoxic respiration (test names ending with _R1).

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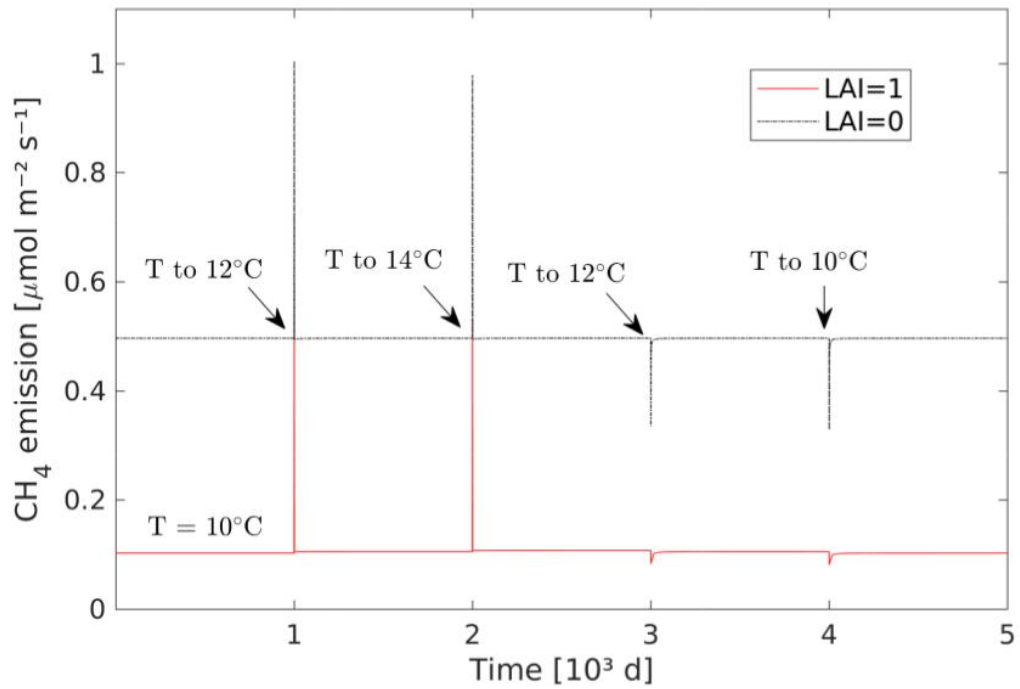


Figure 8. Response of CH₄ emission to changes in peat temperature in the transition tests Ttr W0 L1 (red line) and Ttr W0 L0 (black dashed line) (see Table 3). Black arrows indicate when the input changed.

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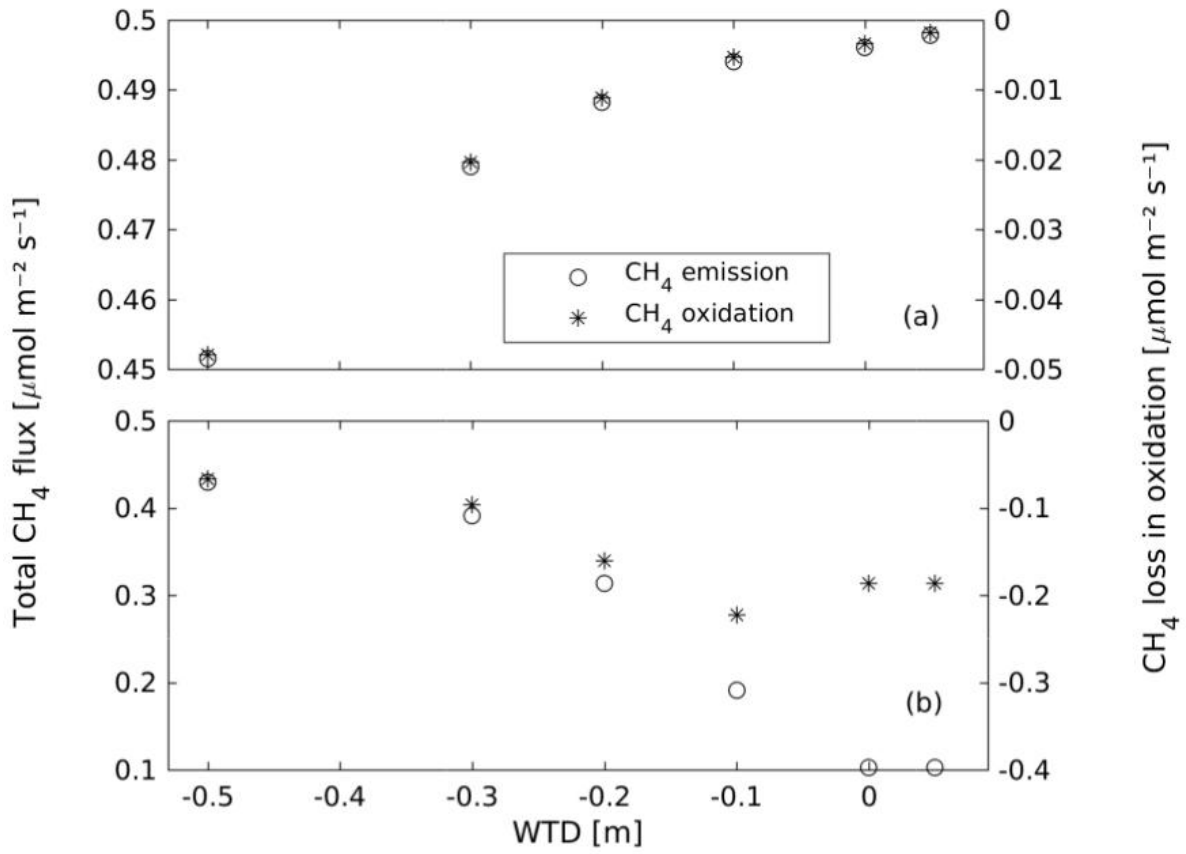


Figure 79. Dependence of the total CH₄ flux and CH₄ oxidation rate on WTD in (a) test W_L0_T10_R1 and (b) test W_L1_T10_R1. CH₄ oxidation is a negative flux since it is loss of CH₄.

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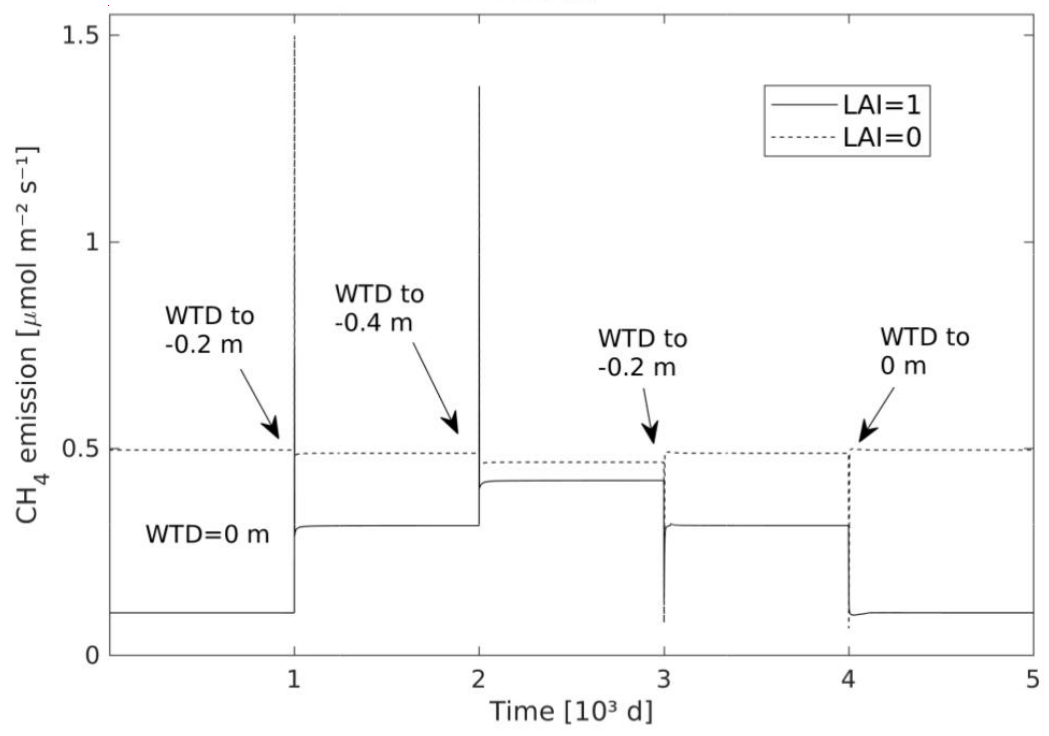
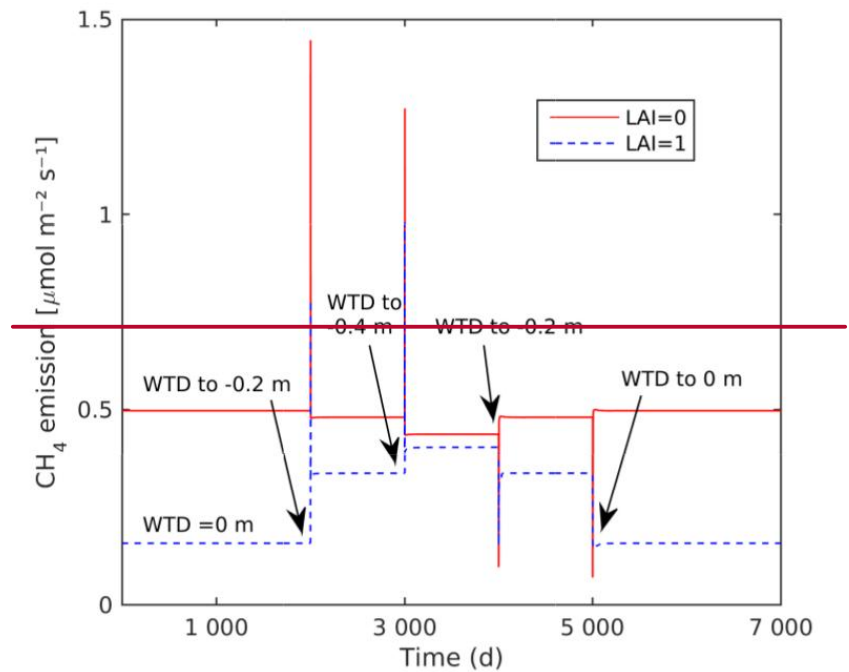


Figure 810. Effect of abrupt changes in WTD on the total output CH₄ emissions in transition tests Wtr_L0 (~~red-dashed~~ line) and Wtr_L1 (~~solidblue-dashed~~ line). Black arrows indicate the change in WTD. This figure also shows how changes in the WTD cause a short ~~artefact~~ peak in the flux, because of how the CH₄ (and CO₂ and O₂) in layers receiving or losing water is handled in the model (see Sect. 3.1.2).

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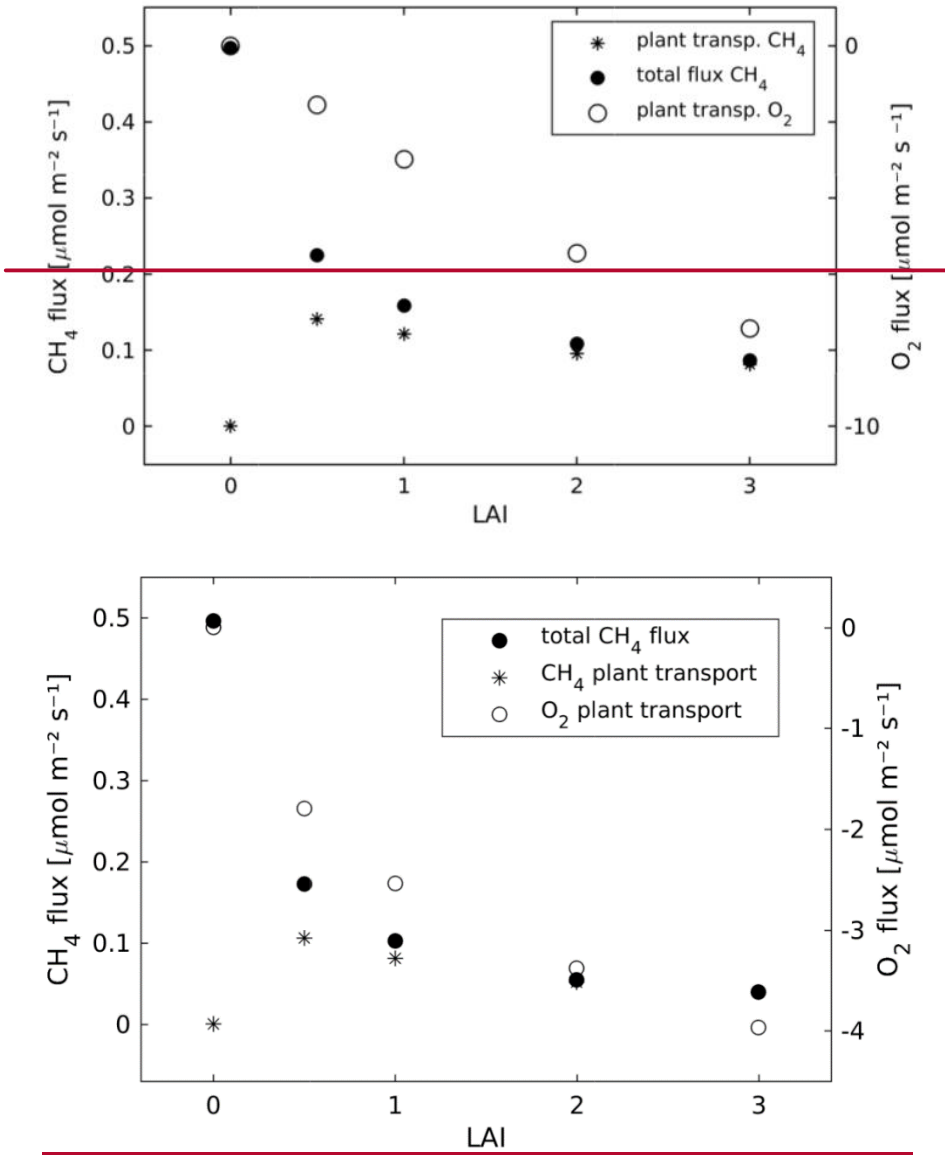
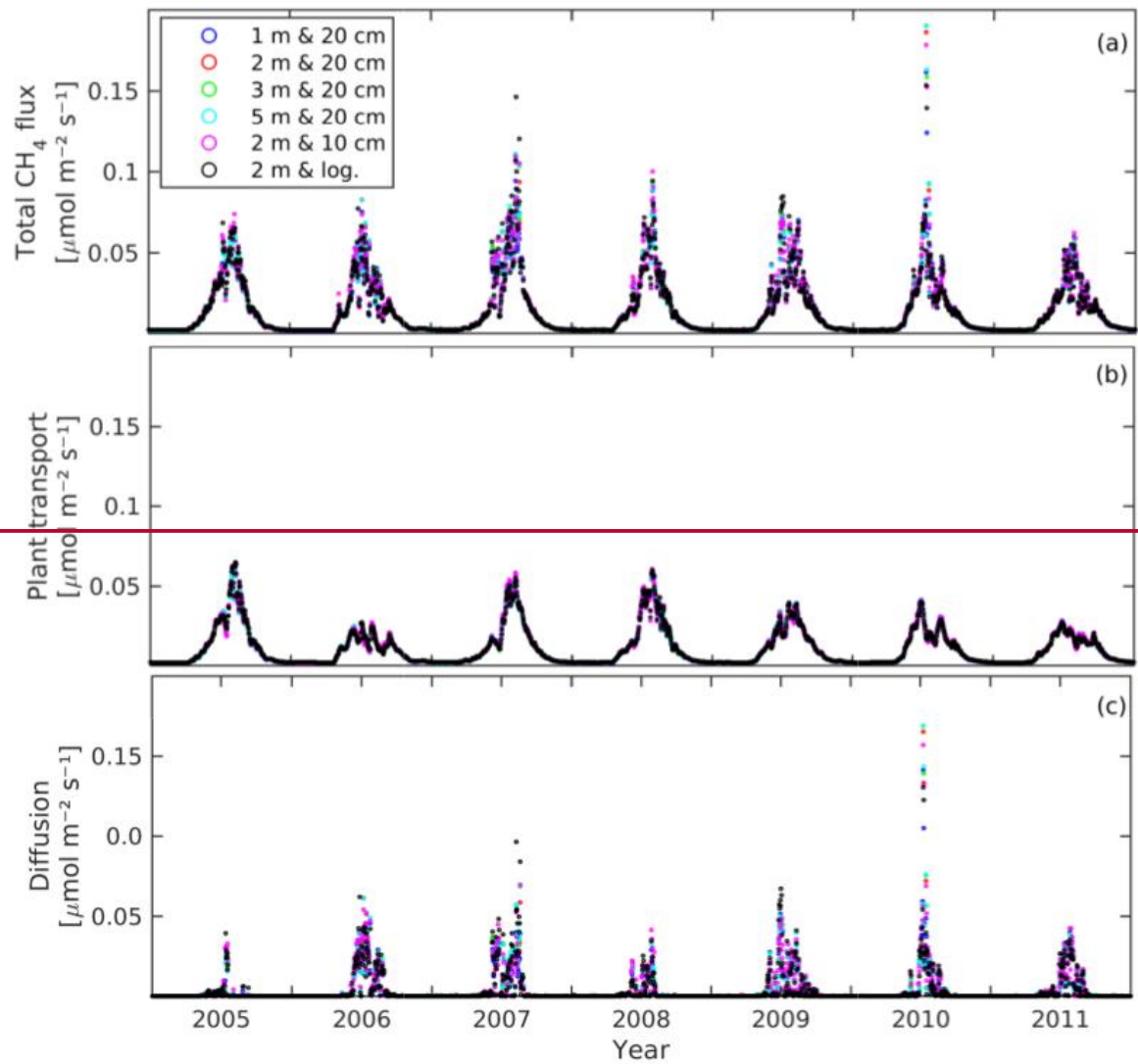


Figure 911. Dependence of total and plant-transported fluxes of CH₄ and plant transport of O₂ on LAI in test L_W0_T10_R1.



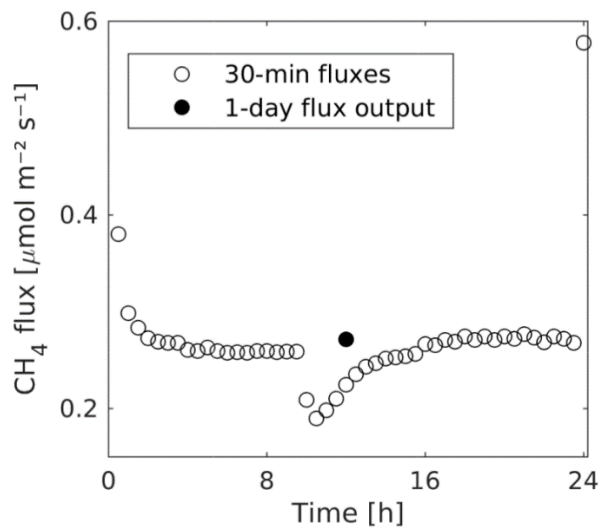


Figure 12. Daily CH₄ flux in the test comparing 30 min and daily time steps.

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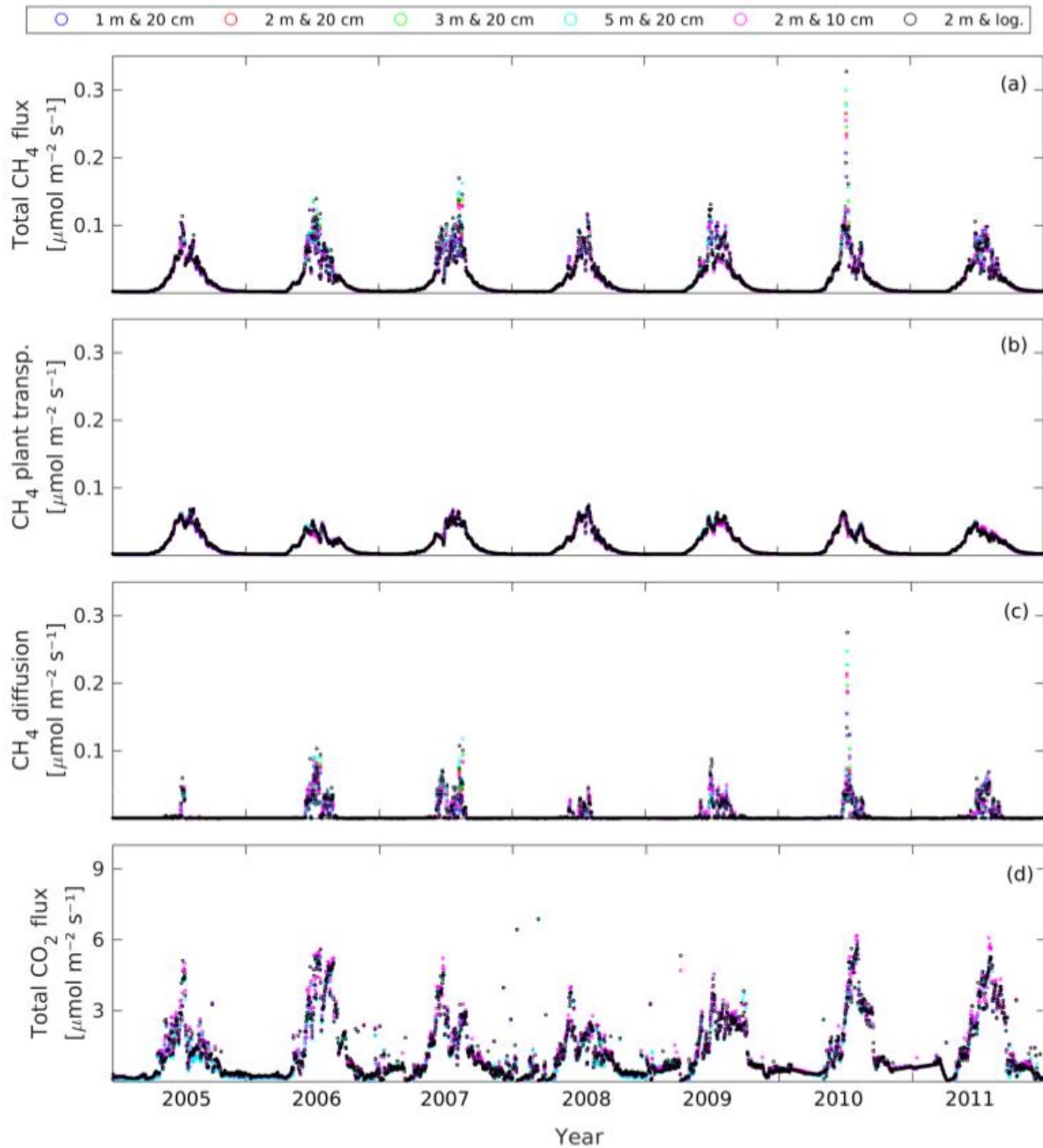


Figure 130. Time series of CH₄ and CO₂ fluxes simulated for Siikaneva in 2005 to 2011, using different peat depths and layer thicknesses with the same input anoxic respiration rate. (a) Total CH₄ flux, (b) CH₄ plant transport, (c) CH₄ diffusion, (d) total CO₂ flux. Direct ebullition to the atmosphere was negligible and thus not shown. CH₄ ebullited when WTD was below the peat surface was transported to the atmosphere via diffusion in peat or plant roots.

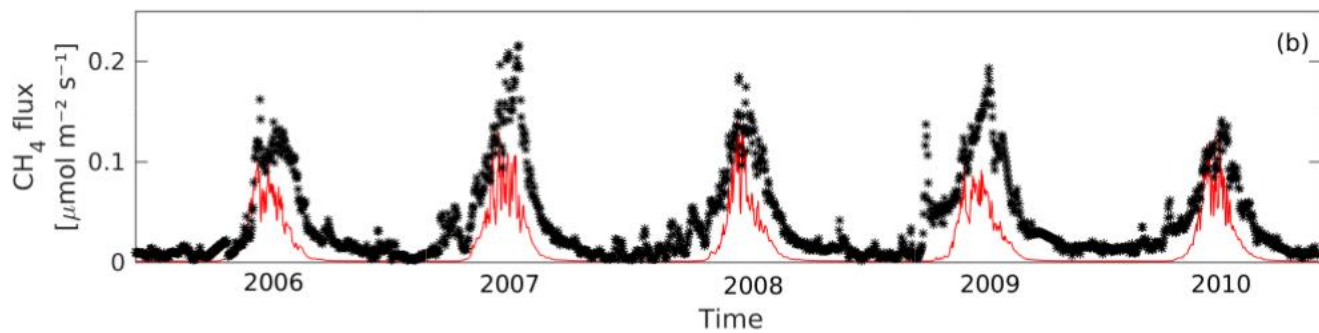
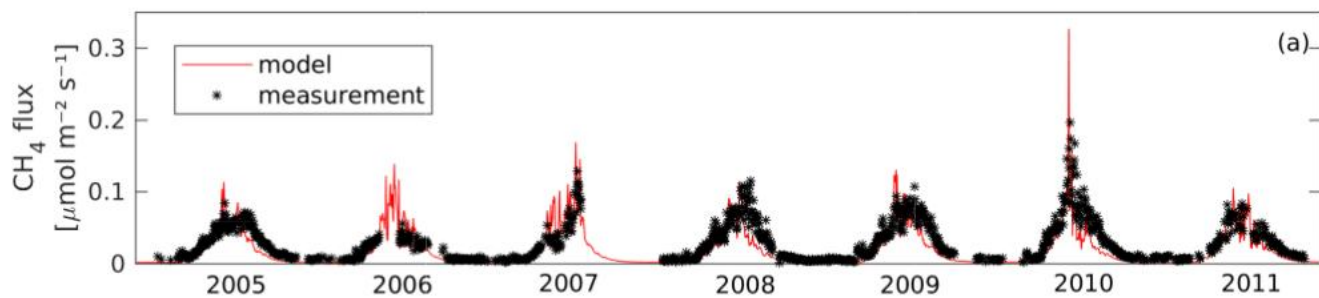
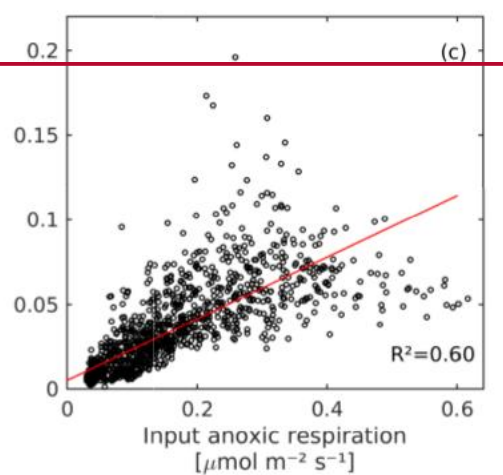
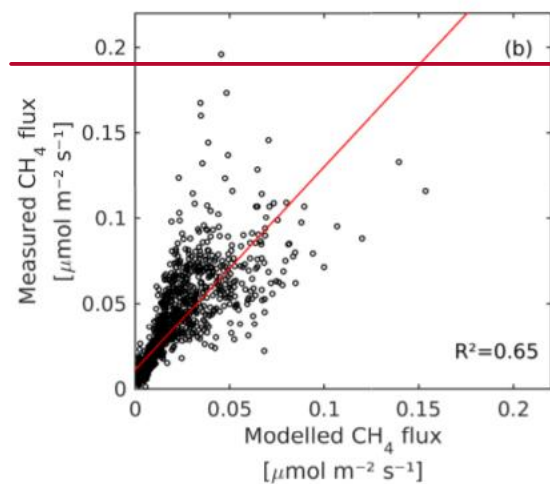
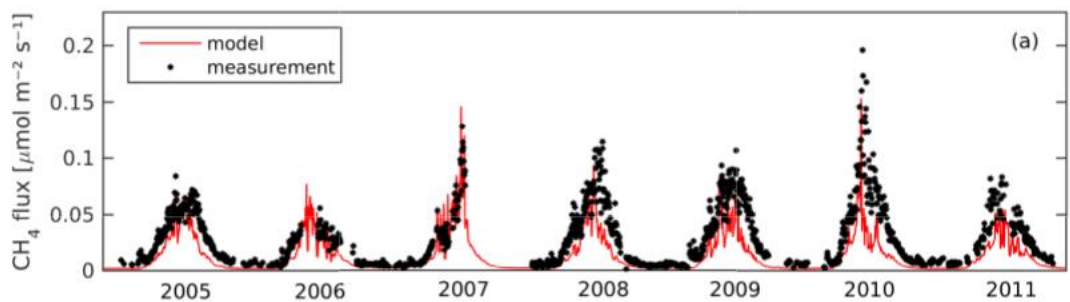


Figure 14. Comparison of simulated and measured CH₄ emissions (a) at Siikaneva and (b) at Lompolojänkkä. The simulations used the logarithmic layer structure and 2 m of peat.

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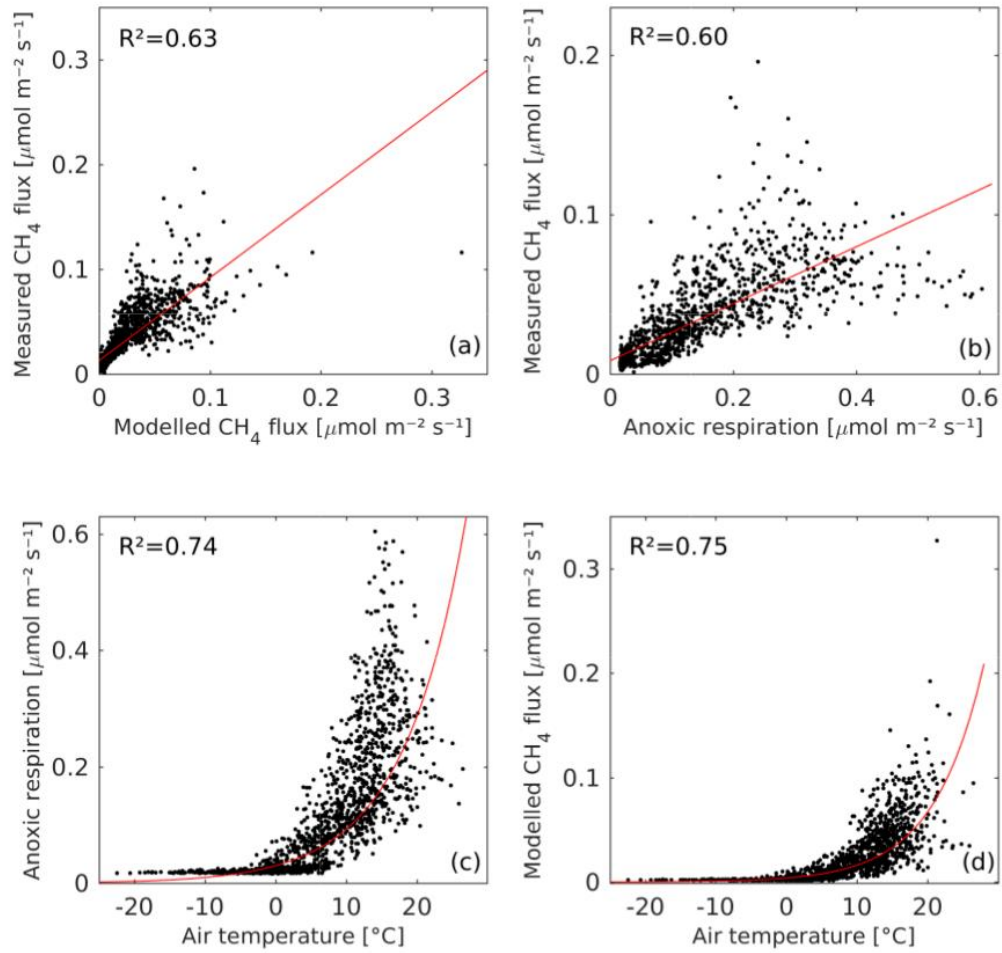


Figure 11.5. Comparison of the measured and modelled CH₄ fluxes of Siikaneva. The modelled flux is from the simulation with logarithmic layer structure and 2 m of peat, driven with measured temperature profile and WTD and simulated LAI and anoxic respiration. (a) The time series of measurements versus model, (b) correlation between model and measurement, (c) correlation between the anoxic respiration rate given as input to the model and the measured CH₄ fluxes, (d) observed air temperature and input anoxic respiration, and (e) observed air temperature and modelled CH₄ flux. The data are from the Siikaneva test (Fig. 14 a).