bg-2021-259

Technical corrections

We would like to thank the editor and the referees for the effort and time they put into reviewing our manuscript. We have considered and addressed the comments in the revised manuscript and corrected or otherwise clarified the issues that the editor and the referees had raised.
In the following list, editor the referee comments are written in bold characters, whereas our responses are shown in regular characters. The line numbers in the referee comments correspond to line numbers in the original version of the manuscript, whereas the line numbers in our responses refer to the revised manuscript.

Response to Associate Editor Decision

Thanks for your revision, which was re-read by both reviewers, who both generally agree that their main concerns have been addressed. Reviewer 1 remains concerns by the lack of focus, and length, of the results and discussion, and provides many helpful suggestions on improving these parts (I would add, re the discussion: try not to restate results!). I agree that these sections are quite long and could be usefully streamlined and on occasion restructured; doing so will help readers and improve the impact of your work. For this reason, please consider and address all of R1's remaining comments, and look for opportunities to tighten the text within reason.

We consider that an extensive discussion on network metrics from the viewpoint of peat structure in Sect. 4.2 is relevant to the aims of the study. The third aim of the study is to assess the capability of complex network theory metrics to describe the physical structure of peat pore space. Also, the title of Sect 4.2 is "Network connectivity metrics related to peat structure and gas transport". Tightening the text would cut down the discussion on one of the main aims of the study. In the revision of the manuscript, we have shifted the main focus from assessment of methane transport capability more towards the description of the physical peat structure by the network metrics as it was suggested by the referees in the first revision round. Because we have introduced the metrics such as closeness centrality and betweenness centrality to the analysis of peat pore structure, we consider that discussion on the applicability of these metrics is justified.

We think that referring to results in question in the Discussion functions as an introductory sentence for the discussion in each paragraph and thus makes the text more readable and comprehensible. This is justified because the network metrics is a new concept in this field of science.

Response to comments from Referee #1

This manuscript has significantly improved in both clarity and motivation after the revisions. The methods are now mostly described with enough detail, and the focus of the manuscript is clearer. This said, however, some reorganization and rewording in the text could significantly increase the impact of the study. The weakest part is the results and discussion where the focus of the study to analyze peat structure to understand gas transport is sometimes completely lost. To make the logic behind the study and the conclusions understandable for a reader who may not be an expert in this field, explaining the meaning of the results in the context of gas transport early on would be helpful. Here below some specific suggestions and comments to try to help with this work.

The focus of the study is not only to analyze peat structure to understand gas transport, but also to analyze the applicability of complex network theory metrics to the description of the physical structure of peat, and this is also discussed in Sect. 4.2 in the Discussion, named as “Network connectivity metrics related to peat structure and gas transport”. We discuss the reasons behind our finding that local and global connectivity metrics do not always properly describe the structure and properties of a peat pore network, which is stated in L412–413 in the manuscript and mentioned also in the Abstract. We think that this is an important issue in the study.

Specific comments:

Line 1: Here it would be helpful if processes leading to CH4 production and transport were separated, so that the reader would get insight why oxygen transport suddenly controls CH4 emissions.

We have clarified the sentence.

L1–2: “The production and emission of CH_4 are strongly influenced by the diffusion of oxygen into the soil and of CH_4 from the soil to the atmosphere, respectively.”

Line 14: Here explaining whether the channel structure affects CH4 transport vs. production would be helpful to guide the reader in how to think about the results.

Here, the discussion on channel structure is focused on the effect on gas transport in general, not specifically on the effect on CH_4. We consider that we already state explicitly in the sentence that channel structure affects gas transport.

Line 18: Please delete word "global". The reader does not yet know what that refers to in this context.

Corrected.

Line 45-50: Please make the connection between gas transport and water retention clear here. Why is water retention an important feature when trying to understand gas transport? This could be done by moving text from lines 60-65 to be earlier.

We consider that the connection between the water retention characteristic and gas transport dynamics is discussed thoroughly in the present paragraph. To make the text clearer, we have moved the first part of the sentence from L62 to the previous paragraph and rephrased the remaining text in L62–63. Further sentence restructuring would break the current structure and flow of the Introduction. We have also clarified the sentence starting from L44.

L44–45: “Water retention characteristic is a fundamental soil property that links soil structure to water dynamics, gas transport, redox conditions, and many accompanying biogeochemical processes (Bachmann and van der Ploeg, 2002; Lepilin et al., 2019).

Line 98: "placed" instead of "located"

Corrected.

Lines 116-120: Please explain why eq (3) was used and why eq (2) was not enough? It seems strange that eq (3) was used even if the fit was not good. It is also unclear which of these equations was used to produce the data in the figures.

The water retention properties of soil are characterized by the water retention characteristic, that is, the functional dependence of volumetric water content on soil matric potential. Water retention characteristic is a fundamental soil property that sets the foundation for water content and energy state and therefore water transport in soil, and essentially affects gas transfer. The functional form of the water retention characteristic is required in all process-based models. Several equations with empirically determined parameters have been proposed to describe the functional form of the water retention characteristic. The van Genuchten parameterization of the water retention curve is widely used in soil science, and the van Genuchten parameters, α and n, can be used to classify soil properties and illustrate the characteristics of a specific soil sample. We have added a short introductory sentence to the description of the model.

Equation (3) was not used for data presentation. The fitted van Genuchten model parameters are only presented in Table 1 for reference and for comparison purposes. We have added references to the equations used in the calculations to the captions of Figs. 3, 4, and 5.

L116–118: “Many empirical models have been constructed to describe the functional form of the water retention characteristic (Hillel, 1998). For comparison purposes, water retention properties were also characterized using the widely used van Genuchten model (van Genuchten, 1980)”.

Line 124: Delete "In short"

Corrected.

Line 125: "With this method..."

Corrected.

Line 126: "obtain" instead of "get"; replace "and" by a comma after "noninvasively"

Corrected.

Line 134: How did you do the reconstruction? How was background subtracted from the CT data?

We have added information on the image reconstruction.

L133: “The conversion of the radiographs to grayscale images was performed with the GE image reconstruction software datos|x.”

Line 141: How did you deal with the separation of the acrylic, please explain briefly so that the reader gets an idea if this method is reasonable.

The separation was performed in a very simple way: a cylindrical region (diameter 1000 voxels) was cropped, that is, selected from the cubical image with horizontal dimensions of 1000 x 1000 voxels. The inner diameter of the acrylic cylinder was 50 mm (1000 voxels), so the cylinder was cut out of the image. We have clarified the wording.

L143–144: “A cylindrical peat volume (height 1000 voxels, diameter 1000 voxels) excluding the acrylic cylinder was selected using PoreSpy.”

Line 146: How did you deal with the challenge that the contrast was low? What error would that induce in your results? Please give an estimate.

The fraction of void space in the image may have been over- or underestimated depending on if the threshold intensity determined for the low-contrast images was too high or too low, respectively. The magnitude of the error is very difficult to estimate. Further, each stage in the workflow from µCT imaging to pore network generation is prone to contain some inherent discrepancy. We find that a thorough analysis of image segmentation and the sources of discrepancy in it is still beyond the scope of this study. We address this issue qualitatively in Discussion: “In addition, the low intensity contrast between air and water or organic matter in the µCT images obscured the determination of the boundaries of the air-filled regions. Generally, this may have had either an increasing or a decreasing effect on the determined air-filled volume. For example, the global solid–void classification method seems to have overestimated the void volume in some of the images of the top layer samples.”

Line 70: Why was it assumed that the sample surfaces were level with the ends of the cylinder? Did you not see that from your samples?

The sample surfaces were probably not totally smooth at the length scale of 50 µm but there was evidently some vertical fluctuation. We have clarified the sentence.

L172–174: “In the calculations, it was assumed that the sample surfaces had been totally smooth and in level with the ends of the acrylic cylinder in the initial, saturated state.”

Line 176: "defined" instead of "assumed"?

In the context of this study and the terminology determined in this section, we set the assumption that there is only one pore cluster extending through the sample domain and refer to it as the pore network. Generally, the number of this kind of clusters is not restricted to one. If there are several this kind of clusters in the sample domain, all of them should be included in the analysis. However, this was not the case in this study.

Line 179: "The volume of the total pore size was..."

Corrected.

Line 184: Does the OpenPNM package use eq 2 or 3 in the calculations? It is hard to understand here what was done with which model of equation and which figure shows results by which method. It is also unclear why all these methods were needed.

The drainage percolation simulation does not use the equations presented in Sect. 2.2, as it simulates the gradual filling of the pore network governed by Eq. (4). The percolation algorithm is described in detail in Sect. 2.7.2.

There are 3 methods in the study. (1) Water retention measurement is a laboratory experiment for the determination of the water retention characteristic of soil, that is, the evolution of volumetric

water content with soil matric potential. (2) Pore network modeling is a method that uses the pore network representation of pore space obtained through μCT imaging and that can be used to simulate water retention and thus to assess the success and performance of the pore network generation process. (3) Parameterization of the water retention characteristic is needed, for example, for the description of soil water retention in biogeochemical models, and the parameters of the van Genuchten model can be used to characterize the water retention properties of soil. The model also presents a functional form of the water retention characteristic.

All the measured volumetric water content and air-filled porosity values presented in this study were obtained with Eqs. (1) and (2), and all the simulation results for the evolution of air-filled porosity with matric potential were obtained with the drainage percolation algorithm of the OpenPNM package. The van Genuchten parameters are only presented, for reference, in Table 1.

We have added an introductory sentence in Sect.2.7.2.

L186–187: “We used pore network modeling to assess the performance of the pore network approach against the measured water retention properties and to perform further simulations in the peat pore networks.”

Line 203: does the "slight vertical shrinkage" here refer to shrinkage during imaging, or some other stage of the experiment? Were the samples imaged after each pressure that was applied to them?

The shrinkage refers to the shrinkage with decreasing volumetric water content during the water retention experiment. To clarify the issue, we have mentioned in Sect. 2.3, which describes the imaging procedure, that the imaging was performed after the retention experiment.

L131–132: “After the water retention experiment, the soil samples [...] The samples were at -10 kPa matric potential during the imaging.”

Line 214: delete "better"

Corrected.

Line 234: Please include the text below in the same paragraph as the text above. the topic doesn't really change here.

Corrected.

Line 258: Please indicate which equation was used for calculating the results presented here.

The equations (1) and (2) for volumetric water content and total porosity, respectively, were used, and the air-filled porosity was calculated by subtracting the volumetric water content from the total porosity. We have clarified the sentence.

Line 259-261: Why is it important to state the percentages here?

The shrinkage percentages illustrate the size and shape of the samples during imaging, at -10 kPa matric potential. As it is seen later in the results and discussion, peat shrinkage had a large effect on the performance of μCT imaging and on the performance of the pore network extraction and pore

network simulation methods. Also, the results of the shrinkage measurement described in Sect. 2.2 are presented here.

Line 262-263: This sentence seems like it explains the reason behind the first statement. Please reorganize.

The sentence does not refer to the previous statement but is an introduction for the following sentences.

Line 265: Please add "measured void space" to indicate whether the discussion is about modeled or measured values.

The sentence does not refer to the air-filled volume determined through water retention measurements but to the void space volume calculated from the binary (solid–void) images. We have clarified the sentence.

Line 267-268: The last sentence of the paragraph does not seem to be tied to anything. Please reword or delete.

In the determination of terminology in Sect. 2.7.1, we make a general assumption that there is only one cluster (defined as the pore network) extending through the sample domain. In this section (3.1) we state that this was really the case in this study.

L270–272: “The pore networks were the only connected pore clusters that extended vertically through the network domain in each pore system, and therefore, it was justified to use them in the water retention simulations.”

Line 270: Please indicate which method or equation was used for calculating the total porosity here.

There is only one method for the calculation of total porosity of the samples described in the manuscript, Eq. (2). The term “sample porosity” refers to the experimental determination from sample weight and sample volume, “image porosity” or “image void fraction” refers to the fraction of the void voxels in the binary image, and “network porosity” refers to the total volume of the pores in the extracted pore network divided by the network domain volume. All these definitions are found in the text. We have clarified the sentence.

L274: “The total porosity of the peat samples calculated using Eq. (2) differed significantly between sampling depths [...] “

Line 271: does "rather small" refer here to that the difference was too small to have any real-life meaning or consequences?

“Rather small” refers to the fact that the difference was statistically significant but that it was still not very large quantitatively.

Line 280: Please discuss the hysteresis results in more detail. They are mentioned in the abstract and based on that, the reader assumes that they are one of the main results of the study, but here they are mentioned just suddenly in one sentence.

The result in this section, 3.2. are related to the cylindrical network domain and illustrate the hysteresis in these networks, which represent the whole peat samples. Hysteresis also affects the phenomena discussed in Sect. 3.5. We have emphasized in Sect. 3.5 that the hysteresis phenomenon is behind the observed differences in the dynamics of the air-filled volume fraction.

L335–336: “To illustrate the effect of hysteresis, the volume fraction of the connected network was calculated for both imbibition (wetting) and drainage (drying).”

Line 286: Here the term "subsample" that was defined earlier could be actually used.

Corrected.

Line 299: "differed significantly with depth"

Corrected.

Lines 311-315: The results listed here seem very obvious. The text reads as a list of characteristics of peat samples that one woudl assume to obtain without any context and reference for what one should assume. This all could be fixed by moving the text from discussion about implications of anaerobic pocket formation on methane transport to the introduction and forming some hypotheses for what would be expected based on the peat structure.

In our opinion, the results are not obvious. We found that the dependence of pore size on porosity was weaker in deeper layers and that network connectivity did not depend on porosity in deeper layers as much as it did near the soil surface. The depth dependence of the spatial variation of average pore volume is discussed further in the second to last paragraph of Sect. 4.3 in the Discussion. These results are also related to the aim number 3 of the study, which is to assess the capability of network theory metrics to describe the physical structure of peat pore space.

The text in the discussion is not about the implications of anaerobic pocket formation for methane transport but on the implications of pore structure for anaerobic pocket formation and methane production. These issues are part of the results of this study, and therefore, they cannot be presented in the Introduction.

Line 329-335: This section seems to present the most important results in relation to CH4 production and transport. Please consider moving to the beginning of the results.

The larger, cylindrical sample domain is studied in Sects. 3.1 and 3.2, and the smaller, cubical sample domain (subsample) is studied in Sects. 3.3–3.5. Therefore, it is not suitable to move Sect. 3.5 to the beginning of the Results section. In addition, the Sects. 3.1 and 3.2 illustrate and assess the performance of the pore network simulation method by comparing the simulations to experimental results and thus “validates” the applicability of the simulation method, and the further analysis, which is based solely on simulations, then follows in Sect. 3.5. In addition, this section (Sect. 3.5) does not present any results in relation to CH_4 transport as such, as it only discusses the volume available for CH_4 production.

Line 347: Please delete "rather" before "well"

Corrected.

Line 366: Please give an estimate how much this darkening affected your results and how it was dealt with. Were the "false" voids removed by hand?

It is very difficult to give a quantitative estimate of the effect of the darkening on the obtained void fractions of the images. This error only concerns the air-filled porosity estimates of the whole samples presented in Fig. 3 because the top and bottom regions were excluded from the pore network domains. The “false voids” were not always individual regions: the darkening also slightly increased the dimensions of existing void space. Therefore, it was not possible to remove the extra void space by hand. We have now emphasized in the text that the darkening only affected the results presented in Fig. 3.

Line 383: Please give an estimate for how much the peat shrinkage affected the simulations. Does shrinkage here refer to the samples and values obtained from them or something that happens during the simulations?

We consider that the paragraph in question describes the effect of peat shrinkage very thoroughly in a qualitative sense. It is very difficult to give a quantitative estimate. Shrinkage refers to the shrinkage of the samples during the water retention experiment in the laboratory before the μCT imaging. We have clarified the sentence.

L388: “Peat shrinkage during the water retention experiment also affected the results of the water retention simulations.”

Line 388-394: Please indicate whether the discussion here is about imaged data or the other the measurements.

We have clarified the text.

L393–399: “Thus, a fraction of the pore throats that were air-filled in the samples at -3 kPa matric potential may have shrunk so that they were not detectable in the μCT images constructed at -10 kPa matric potential. This may have generated disconnected pore space in the images and decreased the total volume of the extracted pore network. Also, the shrinkage of the samples may have decreased the dimensions of the pore space so that a higher external pressure was needed for air invasion in the simulations. Conversely, the horizontal shrinkage of some of the samples created continuous void space near the cylinder wall at -10 kPa matric potential, and thus the extracted pore network contained pore space that had presumably not been present in the samples at higher matric potential conditions.”

Line 407: Please tell where the result referred to here can be seen, and add a paragraph break after the last sentence on this page.

The sentence (“According to our results…”) was meant to refer to the discussion in the following paragraphs. We have added a reference to Fig. 8. We consider that the last sentence of this paragraph (“The distribution and spatial coverage…”) gives reasons for the previous sentence and serves as a concluding remark for the paragraph and as an introduction to the remaining subsection. We have now emphasized the connection between these two sentences.

Line 410: Please include the paragraph starting on this line to the paragraph above.

See previous comment.

Lines 420-451: This is a lengthy list of findings and feels not connected to the goal of the manuscript. Please consider explaining most of this in the results, so that in the discussion all this can be directly tied to gas transport like in lines 452-462.

The goal of the manuscript is not only to evaluate the network metrics from the point of view of gas transport but also to assess the capability of complex network theory metrics to describe the physical structure of peat (aim number 3 in the Introduction). Thus, we consider that the issues discussed in L427–458 are directly connected to one of the main goals of the manuscript. In the revision of the manuscript, we have shifted the main aims from gas transport and methane production more towards the description of the physical peat structure by the network metrics as it was what the referees suggested in the first revision round. Because we have introduced the network metrics such as closeness centrality and betweenness centrality, we consider that discussion on the nature and applicability of these metrics is justified. Also, we discuss the reasons behind our finding that local and global connectivity metrics do not always properly describe the structure and properties of a peat pore network, which is stated in L412–416.

Line 464: "estimate the diffusion" sounds a bit strong here because no real quantitative estimate is provided. Maybe use word "imply"?

We have changed the word ‘estimate’ to ‘characterize’.

Line 473: Do you mean "does not promote and does not restrain" or " does not promote nut restrains"? The first does not really make any sense.

We meant that the orientation of the diffusion paths is such that gas transfer (1) is not faster in the vertical direction than in the horizontal direction and (2) is not slower in the vertical direction than in the horizontal direction. The main idea was that the orientation of diffusion is isotropic and there is no significant difference in gas transfer rates between different directions. We have clarified the sentence.

L479–480: “According to our results, the orientation of diffusion paths in pore networks is such that it does not restrain gas transfer towards the atmosphere in deeper, more degraded peat layers.”