

bg-2021-259

## Author responses to comments of Referee #2

We would like to thank the referee for the effort and time he put in to comment on our manuscript. We are grateful for his careful and considered comments and will make every attempt to fully address these comments in the revised manuscript.

In the following list, the points raised by the referee are written in bold characters, whereas our responses are shown in regular characters.

The manuscript is a carefully detailed and well described study on pore network analyses of peat soils with a depth differentiated view. The aim is to use results of pore network analyses to help explain methane production potential in these environments. The level of language is very high, the text flow is very good, and it was a great pleasure to review. Although I am not that familiar with micro CT, image analyses and pore network simulations, the results are feasible, while not super surprising, as would be expected from the literature. Still, the manuscript is novel in its approach and comparisons.

I was left a little bewildered, what had happened to the discussion of methane (L371-383 gives some general statements on the importance and general conceptual discussion), in particular, since it was not explicitly modelled nor were the results contrasted against methane flux measurements from the field.

My recommendation is that, now with some distance, the authors re-assess the paper and whether or not the self set aims are fully fulfilled. Perhaps it might be a good idea to focus a little more on the strong technical part of the manuscript and limit the study a little more to the descriptive nature, and then discuss the methane production and diffusion from this vantage points in a more speculative manner. After all, the emerging methane emissions are mostly explained by a conceptual model.

The aim of our work is to study the capability of complex network theory methods and metrics to characterize the physical structure of peat and its pore space and to qualitatively assess the obtained metrics and correlations between them in relation to gas transfer processes in peat. The study also shows the physical existence and evolution of isolated air-filled pockets and illustrates their capability to control the production and emission of gases, and methane in particular, from peat. A more thorough comparison between the pore network modelling method and experimental methods related to gas diffusion efficiency in peat will be the subject of further studies. We will revise and reformulate the study aims in the last paragraph of the Introduction. We will also restructure the Discussion and Conclusions so that the conceptual nature of the assessment of methane-related processes will be indicated more clearly.

Major concern

What does this study have to do with methane emissions? This remained unclear to me. Either, the scope of the study should be a more quantitative

The study is part of a larger project that aims to develop tools for studying and modeling methane emissions from peat. The study aims to create a conceptual basis for the description of processes related to methane generation and its atmospheric emissions. The methods presented and used in this study to assess the structure and connectivity of peat pore space can later be applied to describe the processes related to gas transfer and biogeochemical processes in peat. Specifically, we aim to qualitatively evaluate the potential to use the pore network characteristics revealed by  $\mu$ CT imaging and the complex network theory metrics calculated for these networks for assessing gas transfer and processes related to organic matter degradation in peat. Methane generation generally requires anoxic conditions, and studying the development and evolution of regions prone to anoxia in peat illustrates the capabilities of peat for methane generation. We will revise the aims of the study and restructure the Discussion and Conclusions so that the conceptual nature of the assessment of methane-related processes will be indicated more clearly.

Minor concerns

L5 How can the formation of anaerobic pockets be conceptualized in a pore network approach? This is left unaddressed.

The formation and evolution of pore regions isolated from the atmosphere during peat wetting can be assessed and illustrated using pore network modeling. Performing a porosimetry simulation in a pore network gives a description of the gradual change of the number of air-filled pores and the development of isolated pore clusters. Therefore, a pore network modeling approach offers a way to conceptualize the physical basis of the formation of anaerobic pockets. This is illustrated in the modeling results in Sect. 3.5. We will clarify the issue and reformulate the sentence in the abstract.

L42-43 Here peat specific citations should be made (e.g. Hayward and Clymo (1982), Weber et al., 2017), after all, they suggest a pore size distribution.

We will add the suggested references.

L53 like previous comments.

We will add the suggested references.

L 90 ff section 2.2: was the VGM model fitted to the averages of the replicates from each depth, respectively? Just a minor information to add.

Yes. We will rephrase the description.

L94 Sentence not needed, but not harmful, either.

We will keep the sentence for clarity.

L97 in -> at

We will correct the preposition.

L105 This is a rather bold statement. If samples were not saturated under CO<sub>2</sub> environment of vacuum, my impression is this is not actually correct. Please do not use this assumption.

We did not use the assumption in the calculation of the air-filled porosity of the samples. The mass of the saturated sample was not used in the determination of the total porosity, as the total porosity was calculated using the measured dry mass and an estimated, constant particle density (Eq. 2). Therefore, the assumption that air-filled porosity was zero in the saturated state did not affect the air-filled porosity calculations at other matric potentials. The assumption was only reflected in the fitting of the van Genuchten model, where we state that the value of the saturated water content parameter was assumed to equal the total porosity that we had estimated. In addition, the assumption was used in Fig. 4 as the measured air-filled porosity value at -0.1 kPa matric potential, but this value is not essential in the analysis of the water retention properties presented in the figure. The assumption of full saturation is also consistent with the fact that the pore network was, by definition, filled with water at the initial state of the porosimetry simulation.

Because the assumption is used only for illustrative purposes in Fig. 4, we will remove the statement from this section and state the choice and give reasons for it in the caption of Fig. 4.

L118 quantify the sample: What is meant by this? Please specify.

We meant that the structural properties, such as pore space volume and pore size distributions, can be assessed quantitatively. We will clarify the sentence.

L122 is resolution meant, here?

In tomography, voxel size and (spatial) resolution are different concepts. Voxel size is the spatial dimension represented by one image element. Spatial resolution is related to the size of the smallest distinguishable feature in the image, and it is roughly twice the voxel size in microtomography.

L122 if this is the resolution, then the real micropores <10micron are not resolved. Thus, much of the area where anaerobes may continue to exist is not covered. Please address this limitation in the discussion. This, alongside the problem of dissecting organic from water.

Our study is focused on peatlands or drained peatlands, where the water table depth is less than 1 m. It is therefore assumed that pores less than 30  $\mu\text{m}$  in diameter are essentially water-filled under these conditions. Further, the conceptual discussion on anaerobic pocket formation is not focused on the specific networks analyzed in this study. The argumentation can be generalized to pore networks with any pore dimensions.

Separating water from organic matter was not an issue in this study. The purpose of image segmentation was to identify the air-filled volume of the sample images. The problem concerned dissecting air from other substances than air. The word 'solid' stands for both water and organic

material in the text. The low intensity difference between regions containing gaseous material and regions containing non-gaseous material made it difficult to determine an unambiguous boundary between air and other material. We will clarify the definition of solid in Sect 2.4. and address the role of the low intensity contrast as an error source in the Discussion.

L191 The resulting image

We will correct the sentence.

L198ff you state you exclude the effect of shrinkage (I think you should neglect it in this analyses), but I am not convinced this method does what you say it does. Perhaps elucidate a little more.

We meant that horizontal shrinkage had generated empty space between the sample and the cylinder walls and near the top and bottom of the cylinder. If, for example, we had chosen a cylindrical region with a diameter of 50 mm (cylinder diameter) and a height of 25 mm, it would have included continuous void space generated by shrinkage near the cylinder walls. The selection of a study domain in the middle of the sample ensured that this extra void space was not included in the network domain. We will clarify this point in the description.

L213 relatively? to what?

We meant 'fairly'. We will correct the sentence.

Figure 3: Are the results shown for 3 samples, only, are there replicate samples included in the data? Potentially, including uncertainties in  $x$  might help explain the deviation from the 1:1 line (Table 1). Also, I expect that since the air filled porosity = 0 at saturation assumption is not warranted, the data points would be shifted to the left in  $x$ . This could be explored a little more. Also, what would the intercept in Figure 3 represent?

All the air-filled porosities plotted in the image represent the values at -10 kPa matric potential, and all the seven replicate samples are therefore included in the scatter plot in Fig. 3. We will emphasize this in the figure caption. The  $\mu$ CT imaging of the samples was performed at -10 kPa, and the images correspond to the porosity conditions at -10 kPa. The standard deviations presented in Table 1 are not the uncertainties of individual measurements but show the variation between the replicates at each depth. The assumption that the air-filled porosity was zero at saturation was not used in the determination of the air-filled porosity at -10 kPa. Total porosity was estimated from measured dry bulk density and estimated particle density (Eq. 2 in the manuscript). Air-filled porosity was obtained from volumetric water content (Eq. 1) and total porosity.

L256: "rather coherent": what does this mean, specifically? Contrary to this statement, in Figure 4 I see quite some systematic deviation.

Our description of the correspondence between the simulations and the measurements is indeed rather optimistic. The air-filled porosities derived from measurements and pore network simulations

were rather coherent at different matric potentials for some of the samples, but considerable variation existed between the samples at all depths. We will reformulate the sentence and extend the statement.

Figure 4: exhibits bimodality in the retention curve (i.e. some macroporosity close to saturation) due to sharper drop around 1 cm pressure head. This is visible at the top, and not at the bottom as expected from pedogenesis, again Weber et al. 2017.

In this study, the pore size distributions were obtained and analyzed primarily through the pore network approach, and the larger fraction of macroporosity in the top layer is seen in Fig. 6a. The decrease in individual pore volumes with depth is discussed in Sect. 4.2. We will elaborate this issue and include discussion about the retention curves in the Discussion.

Figure 4: It appears that a normalization was done onto one air filled porosity. correct? If so, please specify.

Absolute, not relative, air-filled porosities are presented in Fig. 4.

Figure 4: why are these simulations not carried out until a pressure head of -100cm? (Same in Figure 5).

As we state in Sect.3.2, the external pressure range used in the simulations extended only to about 3 kPa, which corresponds to the minimum throat diameter of 100  $\mu\text{m}$  detected in the  $\mu\text{CT}$  imaging. The pore networks were therefore emptied of water at a pressure head of -30  $\text{cmH}_2\text{O}$ , and nothing would have happened in the simulations as a result of a further increase in pressure.

L 290: This pattern can, again, be observed in Weber et al. (2017), but also in other sources in the literature. I suggest adding citations, here.

Disappearance of the largest pores and a smaller spatial variability of the pore size distribution in greater depths observed by Weber et al. (2017) can be inferred from Fig. 8a that shows that the variation between the total pore network volume and the number of pores was largest in the top layer and decreased with depth. However, Fig. 8a only indicates that the spatial variation of average pore volume is largest in the top layer. We prefer not to use citations in the Results section. We return to the changes in pore space properties with depth in the Discussion (Sect. 4.2). We will further elaborate this issue and refer to the literature in the Discussion.

L384-385 repetition of introduction

We would prefer to keep this sentence for continuity and as a transition to the subject of the paragraph.

L393: a bit of a leap of faith or perhaps a rather general statement: the simulation provide support for the conceptual understanding to be ok. I think these hard earned results should perhaps be discussed a little more in acknowledgement to this (although I detect absolutely no oversell, here).

We showed that the evolution of isolated air-filled pore space with respect to changes in matric potential was considerably different in drying and wetting. The air-filled pores with no connection to the atmosphere are prone to anoxia. This may give reason to suppose that also the development of anaerobic pockets differs in wetting and drying. The susceptibility of unsaturated peat to anoxia and methane generation is discussed in more length in the previous paragraphs of the section. We will elucidate and justify the argument further in the text.

L425: I see the potential to discuss the obtained pore space characterizing numbers in the light of other peoples results re: methane transport, or any other gas transport in particular. If this does not exist, I suggest to scope this section a little more carefully.

We use geometrical tortuosity as a proxy for diffusion efficiency and assess the applicability of network theory measures to characterize the transport properties of a network by comparing them with geometrical tortuosity. Geometrical tortuosity is, by definition, a direct proxy for network transport efficiency as it illustrates the tortuosity and length of flow paths through a network. Centrality measures (closeness centrality, betweenness centrality) are more advanced metrics adapted from complex network theory. Using geometrical tortuosity as a proxy, we could estimate qualitatively how well the centrality measures and other network theory metrics are able to describe the transport properties of a network. To our knowledge, there are no previous experimental studies on the use of complex network theory metrics for gas transfer in natural porous media. We will reformulate the title and the scope of Sect. 4.3 and emphasize the role of geometric tortuosity as a proxy in performance analysis.

L448 mark you, many of the dead end pores might not have been resolved due to the micro CT technique. Perhaps this should be contextualize, too.

The paragraph concerns the structure of a pore network and the characteristics and possible weaknesses of centrality measures in general, with no reference to a specific realization of a network or the relation of a network to a real porous object it represents. We think that a reference to the specific network is not relevant in the context of this paragraph.

L486: How can a relative quantitative measure (anisotropy) determine the efficiency (a qualitative) absolute measure of gas diffusion.

We did not mean the quantitative performance measure named efficiency but the capability of gas diffusion in different directions. We will change the wording.

## References

Hayward, P. M. and Clymo, R. S.: Profiles of Water Content and Pore Size in Sphagnum and Peat, and their Relation to Peat Bog Ecology, *Proceedings of the Royal Society B: Biological Sciences*, 215, 299–325, <https://doi.org/10.1098/rspb.1982.0044>, 1982.

Weber, T. K. D., Iden, S. C., and Durner, W.: A pore-size classification for peat bogs derived from unsaturated hydraulic properties, *Hydrol. Earth Syst. Sci.*, 21, 6185–6200, <https://doi.org/10.5194/hess-21-6185-2017>, 2017.