Pore network modeling as a tool for determining gas diffusivity in peat



1. Introduction

Peatlands modulate biogeochemical cycles and are globally important carbon stocks. They may become large sources of the greenhouse gases (GHGs) carbon dioxide (CO_2) and methane (CH_4) due to their vulnerability to management practices and changes in climate. Gas exchange between peat and the atmosphere occurs mainly through diffusion, and it is controlled by the structure and connectivity of the peat pore space^[1]. The pore network approach enables an explicit investigation of relations between the physical microstructure of peat and its larger-scale gas transport properties. Pore network modeling (PNM) is an efficient method for investigating the pore-scale processes that affect the GHG dynamics in peat^[2].



Fig. 1. Transverse and longitudinal cross sections of (a, b) the 3D μ CT image of an unsaturated peat sample and (c, d) the 3D binary image showing the void and non-void regions of the sample.

2. Methods

- Cylindrical peat samples (5 cm in height and 5 cm in diameter) from a drained peatland, originally a boreal mesotrophic fen.
- Extraction of macropore (diameter > 100 μm) networks from 3D X-ray micro-computed tomography (μCT) images of the samples (Fig. 1).
- Simulation of steady-state gas diffusion in the pore networks using the open-source PNM package OpenPNM^[3].
- Determination of the soil gas diffusion coefficient (D_s) using the diffusion chamber (Currie) method with different water contents adjusted with a pressure plate apparatus.
- Assessment of the applicability of some traditional gas diffusivity models (GDMs) designed for simplified porous materials or mineral soils.



3. Results

- The measured D_s was lower in deeper peat because of lower air-filled porosity and pore network connectivity.
- Gas diffusivity was not very low even in nearly saturated conditions.
- The simulations reproduced the experimentally determined gas diffusion dynamics rather well, depending on the success of image segmentation and pore network generation (Fig. 2).
- The GDMs were not very successful in estimating D_{s} in peat (Fig. 3).



Fig. 2. Comparison of (a) measurement-derived air-filled porosity (afp) at –3 kPa matric potential (a_{meas}) and the afp of the corresponding pore network (a_{PNM}) and (b) soil gas diffusion coefficients determined from measurements (D_s) and obtained through pore network simulations (D_{PNM}) for the peat samples.



Fig. 3. Measured and GDM-estimated relative diffusivity (D_s/D_0) values against air-filled porosity for peat samples from different depths, Individual values of some of the GDMs are presented by triangular gray markers.

4. Conclusions

- The combination of µCT and PNM is a potential alternative to the determination of D_s through laboratory measurements.
- The simulations and measurements assist in the choice of a proper parameterization of D_s in process-based models that are used to assess GHG dynamics and emissions in peatlands.
- Peat microstructure differs from the structure of the materials for which the GDMs have originally been constructed.
- Ongoing work:
 - Experimental study on CH₄ production in peat cores
 - Transient pore network simulation of CH₄ production and transport processes in peat

Acknowledgements

This research has been supported by the Academy of Finland (project Methane and soil-tree networks: Adding dimensions to greenhouse-gas studies (METNET), grant nos. 325168 & 325169).

References

[1] Kiuru, P., M. Palviainen, T. Grönholm, M. Raivonen, L. Kohl, V. Gauci, I. Urzainki, and A. Laurén (2022), Peat macropore networks – new insights into episodic and hotspot methane emission, Biogeosciences, 19, 1959–1977, <u>https://doi.org/10.5194/bg-19-1959-2022</u>

[2] Kluru, P., M. Palviainen, A. Marchionne, T. Grönholm, M. Raivonen, L. Kohl, and A. Laurén (2022), Pore network modeling as a new tool for determining gas diffusivity in peat, Biogeosciences, 19, 5041–5058, https://doi.org/10.5194/bg-19-5041-2022

[3] Gostick, J., M. Aghighi, J. Hinebaugh, T. Tranter, M. A. Hoeh, H. Day, B. Spellacy, M. H. Sharqawy, A. Bazylak, A. Burns, W. Lehnert, and A. Putz (2016), OpenPNM: A pore network modeling package, Comput. Sci. Eng., 18, 60–74, <u>https://doi.org/10.1109/MCSE.2016.49</u>

Petri Kiuru¹ // Marjo Palviainen² // Arianna Marchionne³ // Tiia Grönholm⁴ // Maarit Raivonen⁵ // Lukas Kohl^{5,6,7} // Annamari Laurén^{1,2}

1: School of Forest Sciences, University of Eastern Finland, Joensuu, Finland // 2: Department of Forest Sciences, University of Helsinki, Finland // 3: Department of Mathematics and Statistics, University of Helsinki, Finland // 4: Finnish Meteorological Institute, Helsinki, Finland // 5: Institute for Atmospheric and Earth System Research (INAR)/Physics, University of Helsinki, Finland // 6: Department of Agricultural Sciences, University of Helsinki, Finland // 7: Department of Environmental and Biological Sciences, University of Eastern Finland, Kuopio, Finland // 7: Department of Environmental and Biological Sciences, University of Eastern Finland, Kuopio, Finland

<u>petri.kiuru@uef.fi</u>