The Potential for Artificial Intelligence to Inform Pore-scale Patterns of Methane Production, Release, and Consumption using Imaging, Real-time Flux Measurements, and Microbial Modeling

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Focal Areas: New methodology/technology; High-resolution automated datasets; Lab ⇔ Field

Scientific and Technical Challenge: The production, release, and consumption of methane are pore-scale processes with global impact. We currently lack the capability to observe and understand pore-scale controls over the methane cycle, e.g., the dynamic role of soil moisture and oxygen content, the configuration of complex pore structures such as "microsites" in soils, and the interplay of different microbial functional groups (e.g., acetogens, acetoclastic and hydrogenotrophic methanogens, methanotrophs). Consequently, models at every scale lack the ability to predict net soil methane emissions at the ecosystem level given the substantial heterogeneities in soil aggregate size, shape, physico-chemical properties, and temporal dynamics.

Rationale: We need a better understanding of how methane is produced within and released from soils, but there are numerous complexities that have thus far inhibited understanding and prediction of gross and net methane fluxes from soils. Methane production (methanogenesis) and consumption (methanotrophy) occur in soil pores, where heterogeneities in pore size and configuration control O_2 levels and moisture content (Silver et al. 1999). Methanogenesis is restricted to anaerobic conditions, that can develop rapidly in response to increases in soil moisture, and can also persist in microsites long after soil macropores have drained and reoxygenated. Changes in moisture can differentially affect substrate supply for acetoclastic methanogens (solute substrate) and hydrogenotrophic methanogens (gas substrate) (Sihi et al. 2021). Methanotrophs tend to thrive in aerobic conditions, but aerobic conditions can also persist inside microsites, fueling the consumption of methane even under anaerobic conditions. The advent of technologies for simultaneous measurement of methane and carbon dioxide in automated flux chambers has greatly increased the ability to observe high-resolution temporal dynamics (O'Connell et al. 2018, 2022; Bond-Lamberty et al. 2020 [CO_2 only]). These kinds of surface soil measurements can constrain net methane fluxes, but the complexity and spatiotemporal dynamics inside soils remain a mystery that inhibits broader methane predictability. The same principles and techniques needed for methane can also be applied to other redox-sensitive processes like nitrous oxide emissions and metal redox transformations.

Narrative:
Aim 1: Collect imaging and geochemical data under different moisture and O_2 scenarios. The evolution, transport and release dynamics of soil methane can be measured in aggregate-scale microenvironments, and while measurements in cores may be limited to net fluxes, the information content can be greatly improved by high-temporal resolution imaging and spectroscopy. Imaging technologies like CT-scanning and neutron tomography could be used to map soil moisture and gas

content in structured materials such as soil aggregates and cores. Neutron imaging could be used to assess methane gas bubble transport rates and resistances within porous media. Bubbles (void space) would be visualized as lighter spots by imaging against a darker background, at scales of 25-150 μm. X-ray CT-scanning could be accomplished on aggregates or mini-cores (diameter ~ 1-2 cm) to provide 20 μm resolution, or with micro-CT resolution of a few μm can be accomplished. Soil cores of 5-10 cm in diameter can be used to better understand processes in macropores and provide correlations with bulk properties such as gas flux, water saturation, and organic C content. Porosity information (pore volume fraction, pore size, and pore connectivity) from imaging can be related to methane storage and release. 3D imaging can be used to reconstruct or track a bubble as it migrates through time, at scales of sub-μm to mm. Imaging may also identify active microorganisms indicative of "hot spots" of activity. At the smallest scales, synchrotron spectroscopy can identify metal redox species in the solid phase which can be key indicators of the redox environment and can alter the direction and outcomes of redox reactions, i.e., iron and sulfate reduction can inhibit methanogenesis (Bear et al. 2021).

Aim 2: Configure AI models to match imaging, geochemical, and methane flux data. Convolutional neural network (CNN) can be used to learn the relationship between the soil structure and methane fluxes, soil moisture and O_2 content (Liu et al. 2022). For data gaps, AI can generate new images to fill the gap, using generative models such as GAN for normalizing flow and diffusion models. There are also ML models for feature extraction, segmentation, and clustering; these can be used to guide and optimize image segmentation during CT or neutron scanning (e.g., Venkatakrishnan et al. 2021). We can use a regionalized CNN model for image segmentation to extract interesting features and learn the pore volume in the soil core from the image, and also learn the relationship between the pore volume and the methane flux, moisture and O_2 content. For time series data, we can use long short-term memory network; if the data is an image, we can use CNN; if the data is like a network containing both spatio-temporal information, we can use graph neural network.

Aim 3: Allow AI model to constrain the processes in the model and provide parameters for different scenarios. We can use AI to test and parameterize existing models (Xu et al. 2015, Sihi et al. 2021) that contain key mechanisms such as acetoclastic and hydrogenotrophic methanogens, methanotrophs, acetogens, dissolved organic carbon supply, sulfate concentrations, O_2 concentrations, and pH changes. Other measured constraints such as Eh and other alternative electron acceptors could be used to help aid in convergence of the AI and microbial functional models. ML models can facilitate process-based model simulations by building a fast-to-evaluate surrogate model to reduce computational cost of the process-based model to facilitate parameter estimation or uncertainty quantification. Invertible neural networks can be used to build a surrogate model and estimate the model parameters at the same time as the process-based models, thereby permitting convergence between process- and ML-models.

Aim 4: Match the trained AI model to complex field- and lab-scale data to enable site-level predictions and beyond. Scaling up, the trained AI model could be used to match existing automated chamber data at lab and field scales (O'Connell et al. 2018, 2021; Sihi et al. 2021; new datastreams at the SPRUCE experiment). When connected with time series data such as soil moisture, O_2, methane fluxes, Eh, etc., interpretable ML models can help explain the importance of various drivers and their contributions to bulk methane flux predictions from the field. We can quantify the uncertainty of both the ML and process-based model, analyze the contribution of prediction uncertainty from the model structure, model parameter and data, and use this uncertainty analysis to guide data collection and further improve model development. Finally, ML can assist with multi-scale modeling to extrapolate learning to sites lacking imaging and pore-scale data. This project would provide new insights into key microsite dynamics and improve the prediction and controls over net methane fluxes in soils.

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