Merging top-down and bottom-up estimated wetland CH4 emissions using AI/ML

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Focal Area(s): This white paper is consistent with focal areas 3: when successful, this effort will identify the key mechanisms that govern CH4 wetland emissions and bridge the gap between top-down and bottom-up estimations**.**

Science Challenge: Large discrepancies exist in global CH4 emission estimations between bottom-up and top-down methods. Since 2012, global CH4 emissions have been tracking the warmest scenarios assessed by the IPCC. Bottom-up methods suggest almost 30 % larger global emissions (737 Tg CH4 /yr, range 594–881) than top-down inversion methods. The most important source of uncertainty in the methane budget is attributable to natural emissions, especially those from wetlands and other inland waters (Saunois, et al., 2020). AI/ML has successfully brought observational data's insights into model parameterization and calibration. With the accumulation of available flux measurements, there is an opportunity to **use AI/ML to bridge the gap between top-down and bottom-up estimated wetland CH4 emissions.**

Rationale: There are numerous factors that contribute to the uncertainty in process-based estimates of CH4 emissions from wetlands, including model structures, assumptions, parameterization, and selection of forcing data. However, among these sources of uncertainty, the lack of CH4 flux measurements is a particularly significant factor. In addition, the sensitivity of CH4 fluxes to environmental controls is not well understood, which also limits explicit representations of many mechanistic processes in models. Top-down methods assimilate atmospheric CH4 data and have better constraints on the emission estimations, but they can only obtain a budget-level estimation of CH4 emissions without additional information. Our hypothesis is that unknown mechanistic processes hamper the convergence of the top-down and bottom-up CH4 estimations.

Narrative: Large discrepancies exist in global CH4 emission estimations between bottom-up and top-down methods. With improved partition wetlands and other inland waters, wetland emissions are about 35 Tg CH4 /yr lower than previously published budgets (Saunois et al., 2016; Kirschke et al., 2013). However, the overall discrepancy between bottom-up and top-down estimates has been reduced by only 5 % compared to Saunois et al. (2016), due to a higher estimate of emissions from inland waters, highlighting the urgent need for an understanding of the mechanisms governing wetland methane emissions.

The bottom-up estimated CH4 fluxes range from simple empirical models to detailed process-based model simulations, providing the prior fluxes for top-down estimations. A process-based model is also the land component of an Earth System model and directly drives climate projections. Previous simulations using process-based models have shown a significant level of uncertainty in estimating wetland CH4 emissions at regional and global scales. This uncertainty can be attributed to several factors such as the model structures, assumptions, parameterization, and choice of forcing data. Moreover, the impacts of environmental factors on CH4 fluxes are not entirely clear, which further restricts the explicit representation of various mechanistic processes in the models.

CH4 wetland emissions are inextricably linked to hydrology. Accordingly, there is considerable intra- and inter-annual variation in emissions in response to variations in precipitation and groundwater. CH4 model studies face a significant challenge in capturing the complex interactions among climate, soil, and ecosystems. Explicitly representing these interactions in process-based models is difficult without a solid comprehension of the underlying processes.

AI/ML has successfully incorporated insight from observational data into model parameterizations and calibrations. Applying AI/ML to CH4 wetland models' parameters and variables could further improve CH4 emission estimations in the domains of recalibration, bias correction, and uncertainty reduction. It is particularly useful in quantifying the responses of nonlinear processes, like CH4 wetland emissions. With the accumulation of available flux measurements, there is an opportunity to **use AI/ML to bridge the gap between top-down and bottom-up estimated wetland CH4 emissions.**

Firstly, we use AI/ML methods (e.g., feature selection, dimension reduction, surrogate modeling) to find the key environmental control variables and mechanisms that govern CH4 fluxes using eddy covariance flux data and the spatially explicit data of climate, hydrology, and soil properties, e.g., soil moisture, temperature, water table level, water storage, etc.

Secondly, we use AI/ML methods (e.g., smart search, gradient-based, surrogate-assisted, or Bayesian) to optimize the parameters that are associated with key control variables in a CH4 wetland model, CARDAMOM, and correct the CH4 wetland emission biases. Bloom et al. (2017) developed WetCHARTs, a simple, data-driven, ensemble-based model that produces estimates of CH4 wetland emissions based on one heterotrophic-respiration model (CARbon Data Assimilation Model Framework; CARDAMOM) and constrained by observations of precipitation and temperature. CARDAMOM/WetCHARTs will serve as a working surrogate for an Earth System compliant land model, necessary for us to use here building the AI/ML capability.

Thirdly, we link atmospheric CH4 concentrations with CH4 emissions through an atmospheric transport model and investigate governing processes that affect the temporal and spatial variations of atmospheric CH4 concentrations. This step could possibly be done by spatiotemporal pattern recognition, AI/ML-based error modeling, and physics-informed AI/ML. The key is to determine the source region of measured atmospheric CH4 concentrations.

The workflow will be modularized to be easily transferable and generalizable, and efficiently deployable for any terrestrial biogeochemistry model, such as the E3SM land model (ELM).

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