7-13-2021

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JGR Biogeosciences

RESEARCH ARTICLE
10.1029/2019JG005468

This article is a companion to Yuan et al. (2021), https://doi.org/10.1029/2020JG005963.

Key Points:

- A new CH_4 module was integrated into an Earth system model to predict CH_4 fluxes in a northern Minnesota peatland
- The model accurately predicts the seasonal cycle of methane production and net fluxes
- CH_4 substrate and production were the most critical mechanisms regulating temporal patterns of CH_4 fluxes

Supporting Information:

Supporting Information may be found in the online version of this article.

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Citation:

Ricciuto, D. M., Xu, X., Shi, X., Wang, Y., Song, X., Schadt, C. W., et al. (2021). An integrative model for soil biogeochemistry and methane processes: I. Model structure and sensitivity analysis. *Journal of Geophysical Research: Biogeosciences*, *126*, e2019JG005468. https://doi.org/10.1029/2019JG005468

Received 20 SEP 2019
Accepted 4 AUG 2020

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Abstract Environmental changes are anticipated to generate substantial impacts on carbon cycling in peatlands, affecting terrestrial-climate feedbacks. Understanding how peatland methane (CH_4) fluxes respond to these changing environments is critical for predicting the magnitude of feedbacks from peatlands to global climate change. To improve predictions of CH_4 fluxes in response to changes such as elevated atmospheric CO_2 concentrations and warming, it is essential for Earth system models to include increased realism to simulate CH_4 processes in a more mechanistic way. To address this need, we incorporated a new microbial-functional group-based CH_4 module into the Energy Exascale Earth System land model (ELM) and tested it with multiple observational data sets at an ombrotrophic peatland bog in northern Minnesota. The model is able to simulate observed land surface CH_4 fluxes and fundamental mechanisms contributing to these throughout the soil profile. The model reproduced the observed vertical distributions of dissolved organic carbon and acetate concentrations. The seasonality of acetoclastic and hydrogenotrophic methanogenesis—two key processes for CH_4 production—and CH_4 concentration along the soil profile were accurately simulated. Meanwhile, the model estimated that plant-mediated transport, diffusion, and ebullition contributed to ~23.5%, 15.0%, and 61.5% of CH_4 transport, respectively. A parameter sensitivity analysis showed that CH_4 substrate and CH_4 production were the most critical mechanisms regulating temporal patterns of surface CH_4 fluxes both under ambient conditions and warming treatments. This knowledge will be used to improve Earth system model predictions of these high-carbon ecosystems from plot to regional scales.

1. Introduction

Northern peatlands contain a vast pool of soil carbon that may be vulnerable to atmospheric release under changing environmental conditions, potentially causing a positive feedback to the climate system (Frolking et al., 2011; Nichols & Peteet, 2019; Yu, 2012). The magnitude of carbon emissions and their mechanistic responses to changing environments are elusive due to the complexity of hydrologic and biogeochemical processes in peatland systems (Blodau, 2002). Methane (CH_4) is one of the key carbon forms leaving peatlands under anaerobic conditions. Given the high radiative warming potential of CH_4 compared to CO_2 (Neubauer & Megonigal, 2015), it is critically important to accurately predict future CH_4 emissions from global peatlands. Peatlands are typically formed over millennial timescales due to organic carbon inputs, long-term water saturation and low temperatures and thus store major amounts of terrestrial carbon (Yu, 2012). It is expected that hydrological and biogeochemical dynamics play important roles affecting CH_4 fluxes from peatlands, but many of these key processes are missing in current Earth system models (Bohn et al., 2015). Therefore, to build a better predictive capacity for CH_4 dynamics in peatlands, it is necessary to fully consider the processes and environmental conditions controlling CH_4 processes, particularly the

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Funding acquisition: Paul J. Hanson
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vertical dynamics of CH_4 substrates, CH_4 production and oxidation, and the CH_4 transport pathways (Xu et al., 2016).

A recent rise in global atmospheric CH_4 concentrations has been attributed to a number of natural and anthropogenic causes, including emissions from peatlands (Nisbet et al., 2019; Poulter et al., 2017; Rigby et al., 2008). While northern peatlands are thought to contribute less than tropical wetlands and anthropogenic sources currently, boreal wetlands have received recent attention in the modeling community due to their larger area, higher warming rates, and high carbon stocks (Bohn et al., 2015). Model predictions in such studies are highly variable, and simple models based on environmental drivers alone (e.g., temperature and water-table height) have relatively poor predictive skill in predicting CH_4 fluxes across a range of ecosystems (Turetsky et al., 2014). Major uncertainties and model biases likely result from poor model representations of CH_4 production, consumption and transport, and a relatively small number of observations for model validation (Bridgham et al., 2013). Uncertainty in the temperature sensitivity of CH_4 production also contributes to prediction uncertainty at regional to global scales (Riley et al., 2011).

The Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment presents a unique opportunity to test model responses against observations under experimentally manipulated environmental conditions at an unprecedented scale within a peatland ecosystem. Specifically, SPRUCE is an experiment in an ombrotrophic bog in northern Minnesota designed to assess the response of northern forested peatland ecosystems to increases in temperature and exposure to elevated atmospheric CO_2 concentrations (Hanson et al., 2016, 2017). The SPRUCE project was designed with a primary objective of providing information and data for model development and improvement. Both direct and indirect effects of these experimental perturbations have already been used to develop and refine new peatland modules within Earth system models (Hanson et al., 2017). In this study, we introduce a new model that integrates multiple sources of pre-treatment SPRUCE data about soil biogeochemistry and CH_4 processes (Xu et al., 2014, 2015) into a processed-based model. The model is further used to answer the following questions:

1. Can our process-based model framework capture pre-treatment observations of CH_4 fluxes, CH_4 concentrations, and associated biogeochemical data within the level of observation uncertainty?
2. Which model parameters and process drive model prediction uncertainty?
3. What pathways dominate CH_4 emissions?

To answer these questions, we developed a new model structure and compare the model results with field-scale observational data. A model parameter sensitivity analysis was used to further examine the behavior of the new model and the most critical parameters and processes contributing to variations in surface CH_4 fluxes under pre-treatment conditions.

2. Methods

2.1. Experimental Site and Data Products

The SPRUCE experiment evaluates the response of the existing peatland biological communities to whole-ecosystem warming up to +9°C at both ambient and elevated (~900 ppm) CO_2 concentrations using open-top enclosures (Hanson et al., 2017). These enclosures are located in a *Picea—Sphagnum* spp. bog (S1 bog) in northern Minnesota, 40 km north of Grand Rapids (47°30.476′ N; 93°27.162′ W; 418 m above mean sea level), in the USDA Forest Service Marcell Experimental Forest (Kolka et al., 2011). The S1 bog is an ombrotrophic peatland with a perched water table that has no groundwater inflow, and it is located at the southern margin of the boreal forest in a sub-boreal climate. It is dominated by a mixed black spruce (*Picea mariana*) and larch forest canopy (*Larix laricina*) with various understory shrubs, including Labrador tea (*Rhododendron groenlandicum*), leatherleaf (*Chamaedaphne calyculata*) and blueberry (*Vaccinium* spp.). Annual precipitation and air temperature average 768 mm and 3.3°C respectively (Sebestyen et al., 2011). The S1 bog was harvested in strip cuts in 1969 and 1974 to test the effects of seeding on the natural regeneration of black spruce (Sebestyen et al., 2011). Ground layer vegetation within the S1 bog is composed of a bryophyte layer dominated by *Sphagnum* spp. mosses but also including feather mosses (*Pleurozium* spp) and haircap mosses (*Polytrichum* spp). The peatland soil is the Greenwood series, a Typic Haplohemist (http://www.websoilsurvey.nrcs.usda.gov), with average peat depths to the Wisconsin glacial-age lake bed of 2–3 m, but depths up to 11 m are present (Parsekian et al., 2012). A further summary of the peat

geochemistry can be found in (Tfaily et al., 2014). Near-surface porewater pH is about 4.0 (Griffiths & Sebestyen, 2016).

The observational, pre-treatment data used in this study were compiled from a number of different research groups that collaborate as part of the SPRUCE project. One set of CH_4 flux observations was measured using a large-collar approach (Hanson et al., 2016, 2017). A second set of CH_4 flux observations was measured using an automatic chamber approach, and was used to validate the model performance (Gill et al., 2017). Meanwhile, surface water and porewater profiles of DOC concentrations were made by Griffiths and Sebestyen (2016); Zalman et al. (2018). The DOC concentration for surface and pore water were from Griffiths et al. (2017). The vertical concentration of CH_4 in the soil profile and soil DOC concentrations were measured are available at the SPRUCE experiment data portal (https://mnspruce.ornl.gov/). In addition to the CH_4-related observations, we also used observations of vegetation growth and productivity to validate model simulations, ensuring the model produces reasonable estimates of vegetation inputs to the soil column. These observations include fine root production and standing crop (Iversen et al., 2017), allometric and biomass data on tree species (Hanson et al., 2012), and *Sphagnum* productivity (Norby & Childs, 2018). Model simulations calibrated using this vegetation information are presented in Griffiths et al. (2017) and Jensen et al. (2018).

2.2. Model Integration and Development

For this study, we implemented a new version of the Energy Exascale Earth System land model (ELM) designed for simulations at the SPRUCE site (hereafter referred to as ELM-SPRUCE). Our site-scale modeling framework explicitly predicts wetland hydrology, allowing for the application of a mechanistic framework that includes representation of the acetoclastic and hydrogenotrophic pathways for methanogenesis and tracks microbial populations in different functional groups. This framework also predicts how methanogenesis and methanotrophy are impacted by local water table and moisture variations. Other modeling groups have developed simulations frameworks with similar levels of mechanistic detail (e.g., Grant, 1998; Hopcroft et al., 2011; Martens et al., 1998; Xu & Tian, 2012), but this is the first application in the Community Land Model (CLM) and ELM frameworks to our knowledge. Our work improves upon CLM4Me (Riley et al., 2011), which is the pre-existing methane model available in ELM and the Community Land Model version 4.5 (CLM4.5), in which gridcell-averaged decomposition rates are used as a basis for computing CH_4 fluxes in inundated gridcell fractions. TECO-SPRUCE, which was also developed for the SPRUCE site, also includes a prognostic water table and CH_4 cycling (Ma et al., 2017), and has been used to assimilate and validate against observations. Both site-specific frameworks allow for a more comprehensive evaluation against available measurements, and the ability to predict potential changes in CH_4 production, consumption and transport related to temperature and CO_2 manipulation. However, our framework adds additional process complexity through its representation of explicit methanogenic pathways and microbial populations.

The new version of ELM-SPRUCE presented in this study integrates previously separate model developments for simulating wetland hydrology (Shi et al., 2015), methane cycling (Xu et al., 2015) and moss plant functional types (Shi et al., 2020; Walker et al., 2017). In addition to this model integration, we incorporate several new developments in this study for simulating wetland biogeochemistry that are described below. For the model integration, we began with the original version of ELM, which branched from the Community Land Model version 4.5 (CLM4.5) (Oleson et al., 2013). In ELM-SPRUCE, we added several improvements were made to meet the specific requirements for the hydrology in the ombrotrophic S1 Bog (Shi et al., 2015), including: revised hydrological parameters, the model representation of hummock and hollow microtopography, and lateral flows. A *Sphagnum* plant functional type incorporating the unique physiology of mosses module was also included (Shi et al., 2020; Walker et al., 2017). Finally, an improved CH_4 module first implemented by Xu et al. (2015) was integrated and further developed for this study. This study specifically focuses on the CH_4 module and its application at the SPRUCE site.

The newly integrated CH_4 module (Xu et al., 2015) replaces the existing CH_4 model in CLM4.5 (Riley et al., 2011) with a more mechanistic representation of biogeochemical processes related to CH_4 cycling. This new module represents CH_4 production and consumption in association with the existing decomposition subroutines in CLM4.5 (Thornton & Rosenbloom, 2005; Thornton et al., 2007). Added processes include DOC fermentation, methanogenesis based on H_2 and CO_2 (hydrogenotrophic methanogenesis),

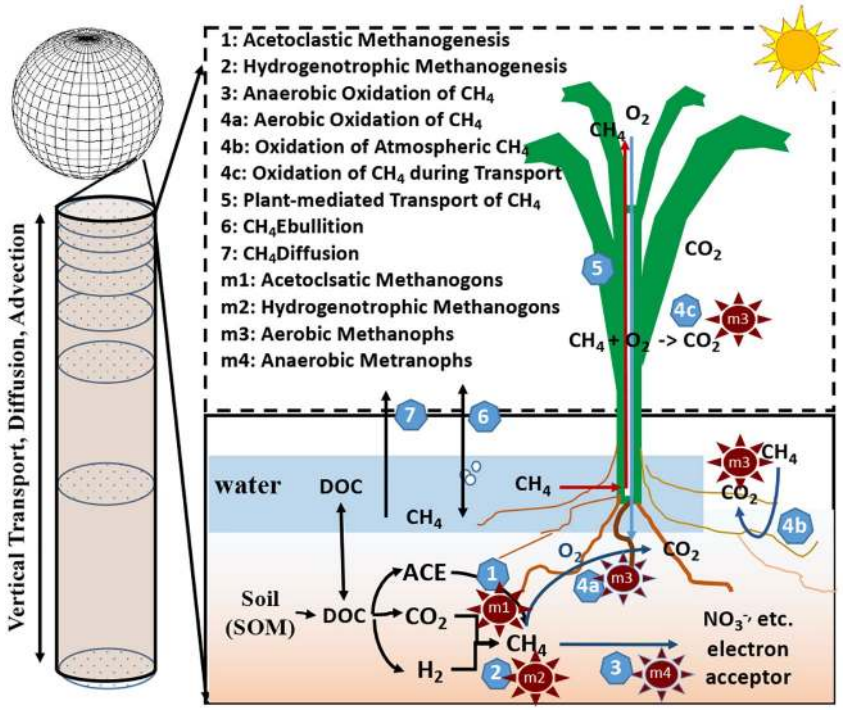

Figure 1. The primary improvements of soil biogeochemistry on the basis of Community Land Model version 4.5 (DOC, dissolved organic carbon; ACE, acetate; the numbers shown in the figure are corresponding to various processes; modified from Xu et al., 2015, 2016).

methanogenesis based on acetate (acetoclastic methanogenesis), aerobic methanotrophy, anaerobic methanotrophy, and H_2 production (Figure 1). All of these mechanistic improvements were developed from known processes (Thauer et al., 1989, 2008), and/or adopted from approaches used in previous modeling studies (Grant, 1998, 1999; Kettunen, 2003; Riley et al., 2011; Segers & Kengen, 1998; Tian et al., 2010; Walter & Heimann, 2000; Zhuang et al., 2004). In addition, this model simulates a pH feedback because acetate formation increases the acidity of soils, which was also observed in incubation experiments (Xu et al., 2015). The detailed information for the CH_4 module, including key parameters and model equations, can be referred in the Supporting Information S1. The simulated surface CH_4 flux is the sum of diffusion, ebullition, and plant aerenchyma-mediated transport. Diffusion is a function of CH_4 concentration and temperature in each layer, ebullition is a function of CH_4 concentration and temperature in each layer; the plant aerenchyma mediated transport is a function of CH_4 concentration, temperature, and root distribution in each layer and the temporal variation of net primary production. The CH_4 concentration is the difference between methanogenesis and methanotrophy; both processes are simulated as a function of microbial biomass, microbial growth efficiency, temperature, soil pH, and oxygen availability (Xu et al., 2015; Wang et al., 2019).

Several further developments to the CH_4 module were undertaken for this study. While Xu et al., (2015) performed CLM4.5 simulations using only one soil layer for the purposes of comparing against incubations, here we integrated the CH_4 modeling into the full 10-layer soil decomposition model for the first time in ELM for the prediction of ecosystem-level responses. This involved adding three new pools for each soil layer: bacterial biomass, fungal biomass, and dissolved organic matter. Each pool has both carbon and nitrogen components. In addition to the 8 pre-existing litter and soil organic matter pools, ELM-SPRUCE now contains a total of 11 pools per soil layer with a total of 34 transitions between different pools and carbon respiration to the atmosphere and nitrogen cycling processes. The processes for carbon flow in and out of bacteria and fungi pools are adopted from (Xu et al., 2014). In addition to these pools, concentrations of dissolved organic carbon (DOC) and acetate are also tracked for each soil layer. Details are included in the Supporting Information S1.

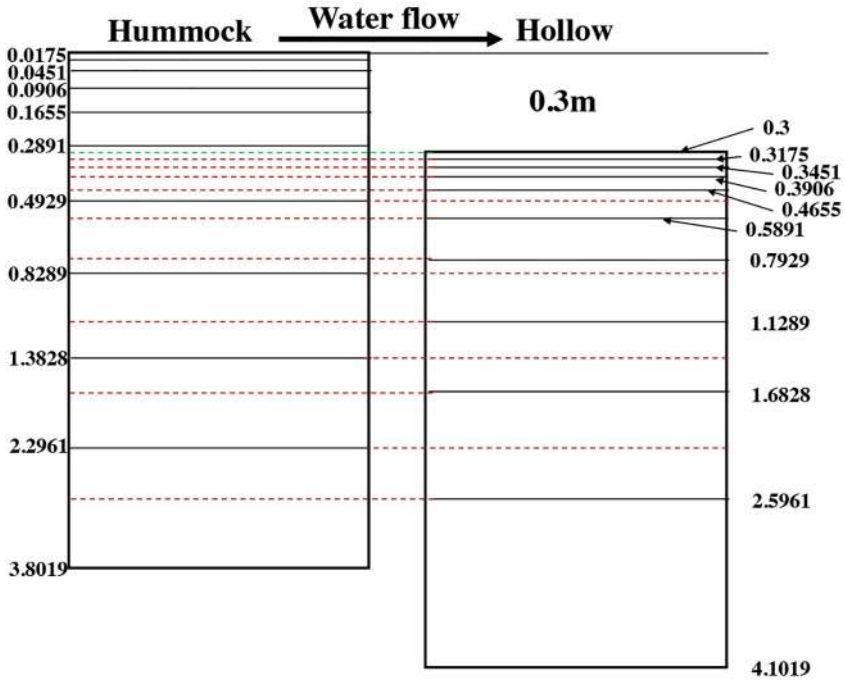

Figure 2. Vertical layer differentiation in hummock and hollow columns for simulating horizontal exchanges of biogeochemical variables (DOC, acetate, CO_2, and CH_4 in this study). Each layer at the same height has horizontal exchange between the columns of biogeochemical variables along a concentration gradient. When multiple layers in one column correspond to one layer in the second column, contributions from each layer are averaged weighted by layer thickness at end of each time step.

We also extend the representation of lateral flows of water within the hummock-hollow microtopography in ELM-SPRUCE (Shi et al., 2015) to include flows of DOC, acetate, CO_2, and CH_4. To estimate biogeochemical processes contributing to CH_4 cycling, the consideration of both lateral and horizontal flows is critical (Cresto-Aleina et al., 2015; Kolka et al., 2011; Verry et al., 2011; Waddington et al., 2015). While Shi et al. (2015) only considered lateral and vertical flows of water in the soil column, we resolve biogeochemical transport and diffusion along these hydrological flow paths. Given our prescribed 30 cm vertical offset between the grid cells, we considered the vertical layers that corresponded to each other on an absolute elevation in the hummock and hollow grid cells. Lateral transport is only allowed between these corresponding layers. Because of the vertical offset between hummock and hollow grid cells, it is not a one-to-one mapping, so that in some cases multiple vertical layers in one grid cell may correspond to one layer in the other (Figure 2) The nutrient and gas concentrations in the new framework were aggregated to a standard vertical profile in ELM-SPRUCE for further calculation or simulation in other modules. The vertical diffusion of DOC, acetate, CO_2, and CH_4 follows Fick's law along the concentration gradient.

The non-methane portions of the model (vegetation and hydrology) variables have been evaluated against observational data from multiple sources. In our previous ELM-SPRUCE study, we evaluated our modeled results for biogeophysical variables such as water table and evapotranspiration (Shi et al., 2015). ELM-SPRUCE simulated net ecosystem exchange is consistent within the uncertainty bounds of pre-treatment carbon budget estimates (Griffiths et al., 2017), and simulated vegetation productivity (Jensen et al., 2018).

2.3. Model Implementation

The model simulations are implemented in a workflow that includes several steps (Figure 3). In the first step, a spin-up simulation is used to generate pre-industrial steady-state values for carbon and nitrogen storage in vegetation and along the soil profile. This stage consists of accelerated decomposition (AD) spin-up and final spin-up following the standard approach of CLM4.5 (Oleson et al., 2013; Thornton & Rosenbloom, 2005). The accelerated spin-up generates an equilibrium state to estimate the relative

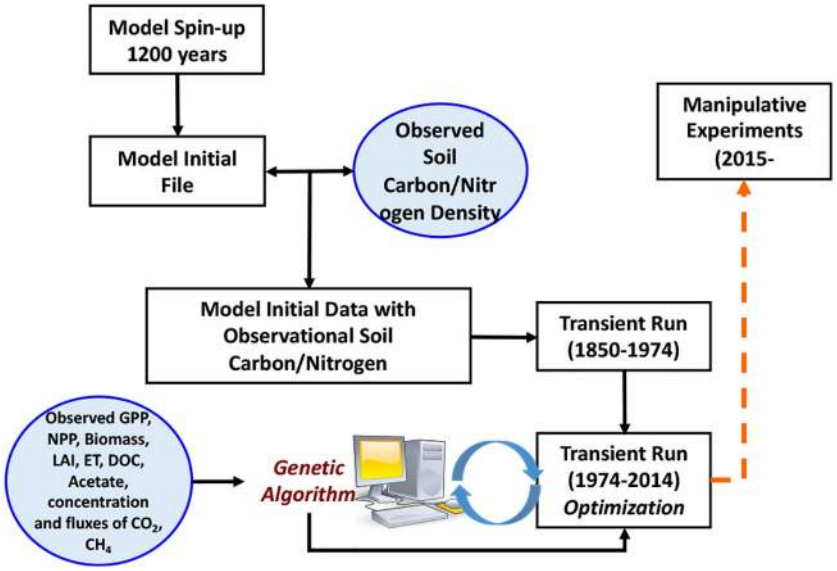

Figure 3. The procedure for model implementation.

content of carbon and nitrogen in different pools including four soil carbon pools and three litter carbon pools, as well as four soil nitrogen pool and three litter nitrogen pools, in each of 10 layers along the soil profile. The length of this AD spin-up is 1200 model years. After readjustment of carbon pools and turnover times following the AD spin-up, a final spin up of 50 years was carried out for re-equilibration. Because the model in its current form is not able to simulate the accumulation of peat, it produces a soil carbon that is, inconsistent with the observed profile. In the second step, after the model spin-up is finished, we re-initialize the soil carbon/nitrogen ratio by adjusting the simulated soil carbon and nitrogen profiles at each soil layer to best match field observations (Iversen et al., 2014; Tfaily et al., 2014). We then adjust the characteristic e-folding depth parameter (Koven et al., 2013) so that our adjustments to the soil carbon profile would not significantly affect the CO_2 emissions from each layer. This procedure allows for a soil carbon profile that is, consistent with observations while maintaining near steady-state fluxes (Table 1). Next, we perform a transient simulation from 1850-1974 in which atmospheric CO_2 concentrations and nitrogen deposition change over time. Finally, we simulate the period from 1974 to 2016, also using time-varying historical CO_2 concentrations and nitrogen deposition. The strip-cut that occurred in 1974 (Perala & Verry, 2011) is represented as a 99% harvest of above-ground tree biomass. In this phase, we also carry out a sensitivity analysis (Section 2.4) and parameter optimization (Section 2.5). After all the model calibration is completed, the optimized parameters are used for a complete set of new simulations from the beginning of spin up and transient runs, including the re-initialization of soil carbon after spin-up. For meteorological inputs for all phases of the simulation, we continuously cycle the observed SPRUCE environmental data (air temperature, wind speed, solar radiation, relative humidity, air pressure, and precipitation) from the period 2011–2017 that were obtained from an environmental monitoring station at the SPRUCE S1 bog (Hanson et al., 2015).

This identical model procedure was repeated for a second version of ELM-SPRUCE, in which the new CH_4 module was turned off and replaced with the default CLM4Me (Riley et al., 2011). This version still uses the Shi et al. (2015) hydrology and microtopography modifications in addition to modifications for the *Sphagnum* plant functional type.

Table 1
The Initial Soil Carbon Pool Size for the Model Transient Simulation Starting in 1974

Soil depth (m)	Soil carbon density (gC m^{-3})	Soil carbon content (gC m^{-2})
0–0.018	22,385	392
0.018–0.045	22,385	617
0.045–0.091	22,385	1018
0.091–0.166	30,294	2271
0.166–0.289	43,978	5436
0.289–0.493	95,584	19,478
0.493–0.829	92,983	31,241
0.829–1.383	83,658	46,341
1.383–2.296	83,799	76,533
2.296–3.802	90,616	63,783

Table 2
Ecological Meanings, Acceptable Ranges, and Optimized Values of the Key Parameters for CH_4 Processes Used in the Sensitivity Analysis and Optimization (Adopted From Xu et al., 2015)

Parameters	Ecological meaning	Minimum	Maximum	Optimal
m_dKAce	Half saturation coefficient of available carbon mineralization	12.8	19.2	16.0
m_dAceProdACmax	Maximum rate for acetate production	1.92×10^{-6}	2.88×10^{-6}	2.48×10^{-6}
m_dH2ProdAcemax	Maximum rate for H_2 production	4.0×10^{-8}	7.0×10^{-8}	6.98×10^{-8}
m_dGrowRH2Methanogens	Hydrogenotrophic methanogen growth rate	8.0×10^{-3}	1.2×10^{-2}	1.0×10^{-2}
m_dDeadRH2Methanogens	Hydrogenotrophic methanogen death rate	8.0×10^{-4}	1.2×10^{-3}	1.0×10^{-3}
m_dGrowRAceMethanogens	Acetoclastic methanogen growth rate	6.4×10^{-3}	9.6×10^{-3}	7.034×10^{-3}
m_dDeadRAceMethanogens	Acetoclastic methanogen death rate	1.6×10^{-3}	2.4×10^{-3}	2.0×10^{-3}
m_dGrowRMethanotrophs	Methanotroph growth rate	6.4×10^{-3}	9.6×10^{-3}	8.0×10^{-3}
m_dDeadRMethanotrophs	Methanotroph death rate	1.6×10^{-3}	2.4×10^{-3}	2.0×10^{-3}
M_dYAOMMethanotrophs	Growth efficiency of anaerobic methanotrophs	0.12	0.18	0.15
m_dACMinQ10	Temperature dependence of acetate production	2.4	3.6	3.024
m_dCH4ProdQ10	Temperature dependence of CH_4 production	1.6	2.4	2.0
m_dCH4OxidQ10	Temperature dependence of CH_4 oxidation	0.96	1.44	1.20
m_dCH4min	Minimum CH_4 solubility	0.04	0.06	0.05
k_dom	Dissolved organic matter turnover rate	5.6×10^{-3}	8.4×10^{-3}	7.004×10^{-3}
k_bacteria	Bacterial turnover rate	0.176	0.264	0.22
k_fungi	Fungal turnover rate	0.176	0.264	0.22
dom_diffus	Diffusion rate of dissolved organic matter	1.44×10^{-7}	2.16×10^{-7}	1.8×10^{-7}
m_dPlantTrans	Efficiency for plant transport of CH_4	5.6×10^{-3}	8.4×10^{-3}	7.0×10^{3}

2.4. Sensitivity Analysis

Model sensitivity analysis is essential for model testing as it helps to apportion different sources of uncertainty in the model parameters or model structure (Cariboni et al., 2007; Haefner, 2005). Here we focus on model parameters, because understanding their sensitivities can provide mechanistic insight into which processes dominate the uncertainty of specific model outputs. A sensitivity analysis was carried out to estimate the model behavior in response to key parameters. In this sensitivity analysis, 19 selected model parameters controlling CH_4 processes were allowed to vary between −20% and +20% from their default values (Table 2). These parameters cover all key processes for CH_4 production, oxidation, and transport through plants, diffusion, and ebullition. We ran an ensemble of 2000 model simulations, randomly varying all parameters simultaneously over their prescribed ranges to identify both the most sensitive and the most stable parameters controlling the CH_4 processes. The computational expense of ELM-SPRUCE is high, requiring about 12 h per simulation on a single processor; therefore, we chose this sampling strategy to facilitate global sensitivity analysis using a surrogate model that is, constructed using Bayesian compressive sensing (Ricciuto et al., 2018; Sargsyan et al., 2014). This approach allowed for sensitivities with high confidence to be obtained with the 2000 model ensemble simulations, a relatively small number for this high-dimensional space. Simulations were performed both with ambient conditions, and +9°C, the highest level of warming the SPRUCE experiment following Griffiths et al. (2017) to understand how the treatments may affect the importance of different processes.

2.5. Model Optimization Algorithm

An evolutionary algorithm, quantum particle swarm optimization (QPSO) (Sun et al., 2004), was used to optimize model parameters related to CH_4 cycling. Because some optimal parameter combinations were identified as unrealistic, we used a manual calibration approach for fine-tuning following the QPSO optimization. Allowable ranges for CH_4 parameters were the same as those used for the sensitivity analysis (Table 2).

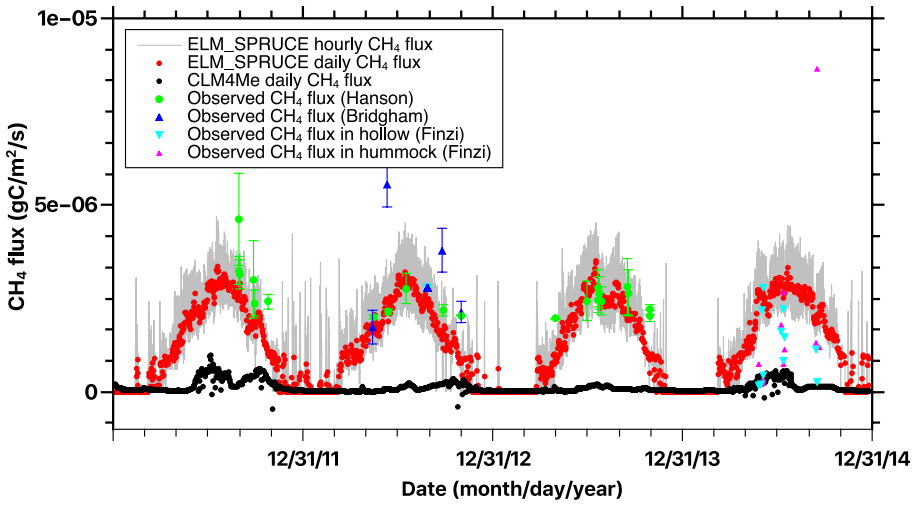

Figure 4. The comparison between modeled CH_4 flux with measured CH_4 from various sources fluxes measured in the field using different techniques.

The QPSO algorithm was used to minimize a cost function, which was constructed using a weighted sum of squared residuals (the difference between model and observation) for all CH_4 related observations described in Section 2.1. Observational uncertainties, when available, were used for the weightings. When uncertainties were not available, we assumed the uncertainty to be 25% of the magnitude of the observed value. Here we used a population size of 50 and 100 iterations to perform the QPSO optimization. The final optimized parameters were the most consistent with the observational data in magnitude and seasonality. Additional fine tuning did not significantly affect the cost function value. More details about the QPSO algorithm and calibration approach are provided in Lu et al. (2017).

3. Results

3.1. Model Validation

In this study, we specifically focus on CH_4 cycling and compare modeled DOC, CH_4 concentration and CH_4 flux against observational data.

The ELM-SPRUCE model is able to capture the temporal variation in land surface CH_4 flux at the S1 bog (Figure 4). The modeled daily CH_4 fluxes display significant correlations with field observations and are well-aligned in terms of seasonality and magnitude ($R^2 = 0.327$; $P = 0.007$; Mod = 0.751 (0.248) × Obs + 2.421E-8 (6.569E-7)) for the large collars (Hanson et al., 2016). Predicting much lower flux magnitudes, the CLM4Me model has an insignificant correlation ($R^2 = 0.112$, $P = 0.137$; Mod = 0.062 (0.040) × Obs + 1.488E-8 (1.056E-7)). The ELM-SPRUCE model also compares well ($R^2 = 0.581$; $P = 0.078$; Mod = 0.089 (0.038) × Obs + 1.427E-6 (3.337E-7)) with the static chamber observations (Zalman et al., 2018), although the small number of measurements means that the results are less statistically significant. The large temporal variations in CH_4 flux from the hummocks and hollows measured using the auto-chamber method (Gill et al., 2017) are less consistent with the daily modeled fluxes ($R^2 < 0.05$). Additionally, while seasonally consistent in relative magnitude, the modeled fluxes were generally larger than the observed CH_4 fluxes from hummocks and hollows; linear regression showed that the modeled fluxes overestimate the auto-chamber observations by about 10%. It is important to note that vegetation was removed in the auto-chambers, which was not considered in these simulations. There is also a timescale mismatch between the point-in-time observation (i.e., a timescale of minutes) and the daily model output. Therefore, the range of modeled hourly CH_4 fluxes, which show higher variability, match better with these measured fluxes. The CLM4Me model did not have significant correlations with the static or autochamber flux data.

We also compared ELM-SPRUCE results to observed vertical profiles of substrates that are important for CH_4 cycling. This further comparison showed that the model can reconstruct the vertical distributions of

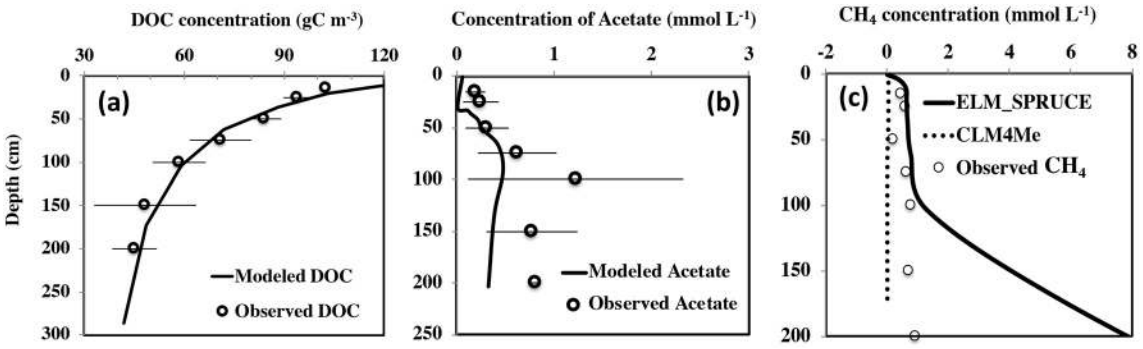

Figure 5. Model comparison with observational data of dissolved organic carbon (DOC), acetate, and CH_4 concentrations along soil profile (the concentration of DOC, acetate, and CH_4 are averages in the 2013 growing season).

DOC ($R^2 = 0.974$; $P < 0.001$; Mod = 0.958 (0.070) × Obs + 6.672 (5.262)) and acetate ($R^2 = 0.588$; $P = 0.044$; Mod = 0.448 (0.168) × Obs + 0.042 (0.116)). For CH_4 concentrations, the model reproduces the data well near the surface but not at depth ($R^2 = 0.06$) (Figure 5). The gradually declining DOC concentration along the soil profile is well-captured by the model in both magnitude and distribution along the vertical profile, and the model is able to simulate the gradual decline in DOC concentration from ~100 to 30 g C m^{-3} at 300 cm depth. The modeled vertical profile of acetate matched well with observed acetate concentration in the top 100 cm of the soil profile, while the modeled acetate concentration is slightly underestimated below 100 cm. The observed CH_4 concentration with depth in the upper meter of the soil profile was simulated, but performed poorly at deeper levels (Figure 5). The CLM4Me does not simulate DOC and acetate, while produces one order lower CH_4 concentration and inconsistent vertical CH_4 profile than the observed CH_4 concentration (Figure 5).

3.2. Sensitivity Analysis

A sensitivity analysis was carried out to estimate the CH_4 emissions and contributions to these emissions from three transport pathways under ambient conditions and under +9°C, the maximum level of warming in the SPRUCE experiment. While we varied 19 model parameters (described in Supporting Information S1), the surface CH_4 flux was sensitive to only five of these parameters—the maximum acetate production rate (*m_dAceProdACmax*), the methanogen growth rate (*m_dGrowRAceMethanogens*), the half-saturation coefficient of available carbon mineralization (*m_dKAce*), the dissolved organic matter turnover rate (*k_dom*), and the methanogen death rate (*m_dDeadRH2Methanogens*). The most sensitive parameter was the maximum production rate of acetate, indicating the importance of substrate regulation for CH_4 production. Under the +9°C warming condition, the contribution of acetate production rate weakened, while the mineralization rate of dissolved organic matter became more important. This shift suggests that while acetoclastic methanogenesis increases with warming, the warming may reduce the role of acetate as a substrate for methanogenesis but enhance the control from DOC, which might be caused by the faster decomposition rate of acetate compared to DOC.

For all three transport pathways, the half saturation coefficient of acetate is equally important. The sensitivities of other key parameters controlling the contribution to CH_4 surface flux from each of three transport pathways are different, providing important information for model parameterization (Figure 6). For example, the most sensitive parameter controlling CH_4 flux from plant-mediated transport under ambient conditions is the substrate production rate, followed by the growth rate of acetoclastic methanogens. Warming increased the sensitivity of the plant transport coefficient (*m_dPlantTrans*). CH_4 flux from the diffusion transport pathway is primarily controlled by the diffusion rate of dissolved organic matter (*dom_diffusion*), which is a key precursor for CH_4 production. The key parameters controlling CH_4 flux from ebullition are the maximum acetate production rate and the growth rate of acetoclastic methanogens. Warming increased the sensitivity of two parameters: the decomposition rate of DOC and plant transport. Shifts in importance among the three transport pathways also resulted in changes to parameter sensitivities for the integrated CH_4 flux at the surface. These sensitivities provide important information about the contributions of model

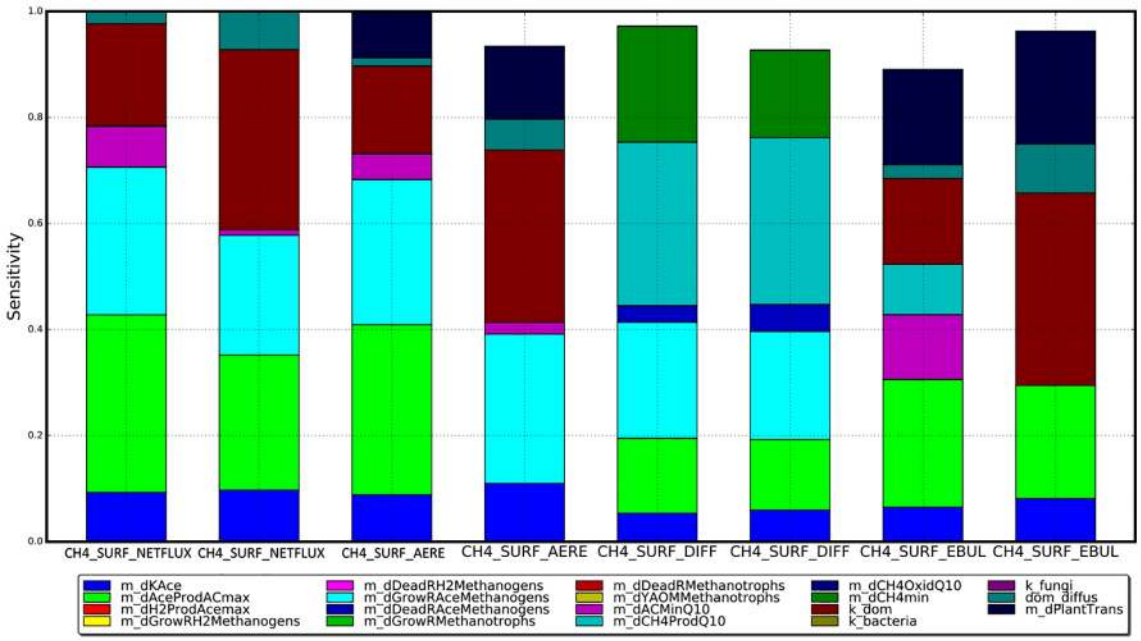

Figure 6. Sensitivity analysis of Energy Exascale Earth System land model-Spruce and Peatland Responses Under Changing Environments parameters for the following model outputs and scenarios: (a) Surface CH_4 flux under ambient conditions, (b) Surface CH_4 flux under the +9°C treatment, (c) Surface CH_4 flux from plant transport under ambient conditions, (d) Surface CH_4 flux from plant transport under the +9°C treatment, (e) Surface CH_4 flux from diffusion under ambient conditions, (f) Surface CH_4 flux from diffusion under the +9°C treatment, (g) Surface CH_4 flux from ebullition under ambient conditions, (h) Surface CH_4 flux from ebullition under the +9°C treatment. The height of each bar indicates the fraction of variance in a model output caused by variations in the corresponding model parameter. Stacked bars sum to one except in cases where higher-order parameter interactions are important (not shown).

processes to prediction uncertainty, and which quantities would be useful to better measure under ambient and warming conditions.

3.3. Modeled Surface CH_4 Flux Along the Three Transport Pathways

The modeled annual CH_4 net efflux from the S1 bog is estimated at 31 g C m^{-2} y^{-1}, close to the calculated annual CH_4 net efflux based on simple interpolation from time series of measured CH_4 flux (Hanson et al., 2016, 2017). The modeled CH_4 flux showed obvious seasonality in plant-mediated transport and ebullition, while the diffusion did not show a clear seasonal pattern (Figure 7). The model estimated that the ebullition, diffusion, and plant-mediated transport contributed approximately 61.5%, 15.0%, and 23.5%, respectively, to the CH_4 emissions to the atmosphere at an annual time scale (Figure 7). There is no modeled CH_4 emission in January, February, and March due to the frozen peat surface based on the assumption that the frozen surface prevents all CH_4 emissions from soil. Because of the buildup of CH_4 beneath these frozen layers, the model simulates an early spring CH_4 pulse when the frozen soil thaws in the spring.

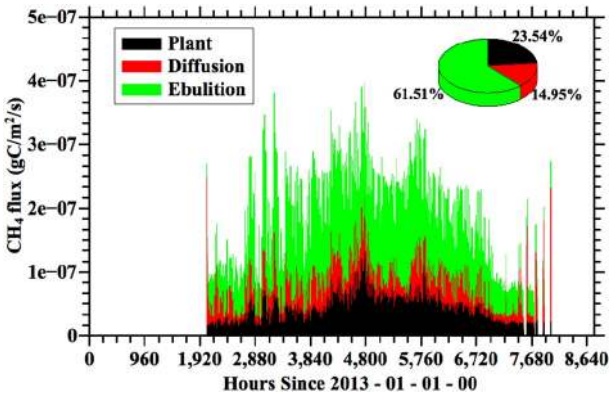

Figure 7. The modeled CH_4 transport pathways and their contributions to the annual budget of CH_4 emission from the S1 bog under ambient condition (hourly step is adopted to better demonstrate the CH_4 dynamic at a high temporal resolution). The pie chart shows the total contribution for each pathway to the annual sum of CH_4 emissions.

3.4. Differences Caused by Microtopography

Hummock and hollows are unique microtopographical features in peatland ecosystems. ELM-SPRUCE assumes a 0.3 m elevational difference between two adjacent grids to represent a "mean hummock" and a "mean hollow." The simulated surface CH_4 flux and water table dynamics are

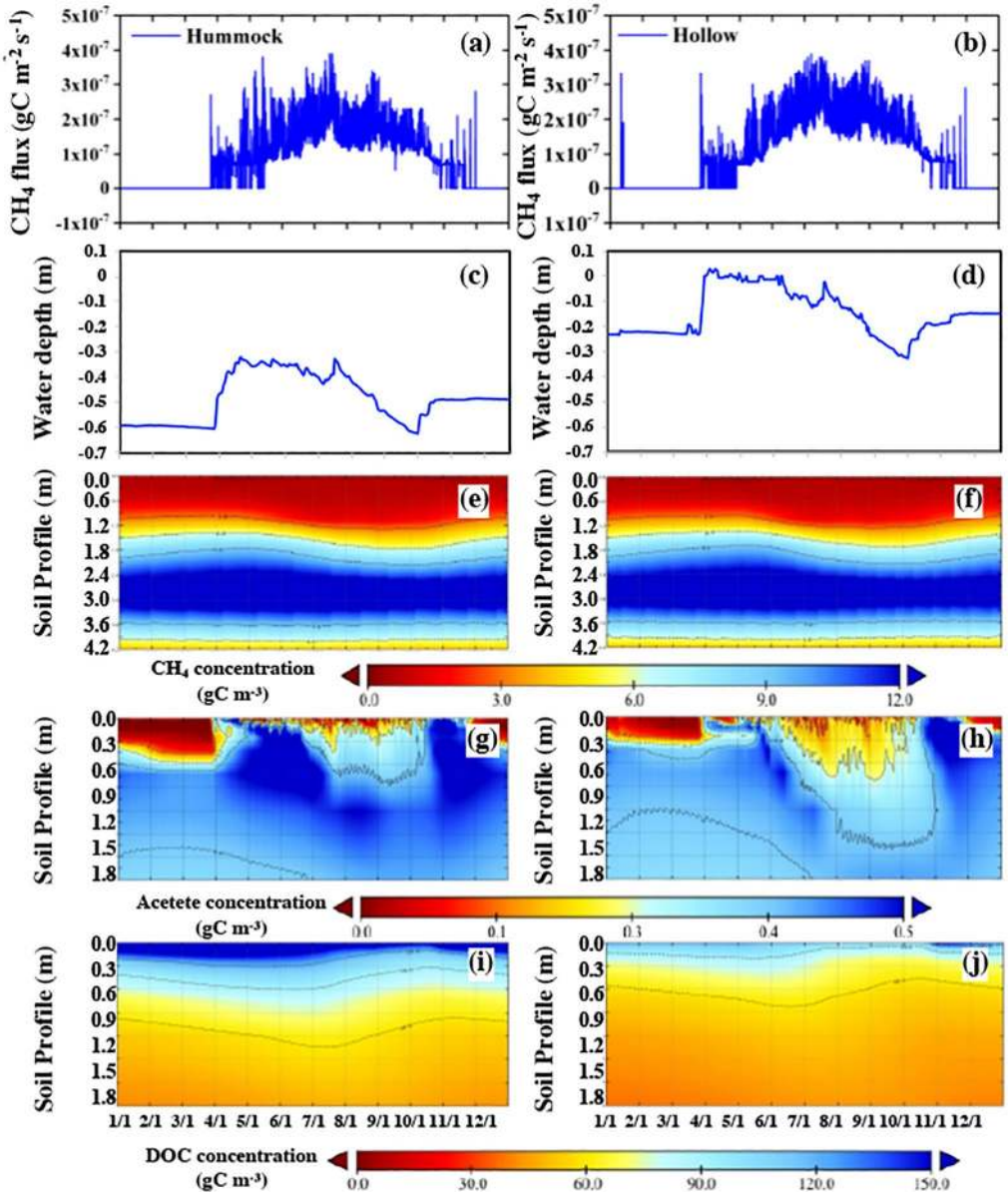

Figure 8. Seasonality in the vertical profiles of dissolved organic carbon (DOC), acetate, and CH_4 concentration and their resultant surface CH_4 flux and surface water table dynamics for hummock and hollow columns in 2013 (a) Surface CH_4 flux from hummocks; (b) Surface CH_4 flux from hollows; (c) Water table dynamics in hummocks; (d) Water table dynamics in hollows; (e) Soil/water profile of CH_4 concentration in hummocks; (f) Soil/water profile of CH_4 concentration in hollows; (g) Soil/water profile of acetate concentration in hummocks; (h) Soil/water profile of acetate concentration in hollows; (i) Soil/water profile of DOC concentration in hummocks; (j) Soil/water profile of DOC concentration in hollows; notice the difference in the *Y*-axis scale for water table between panels (c) and (d).

only slightly different, while the belowground hydrology and biogeochemistry are different for hummock and hollow (Figure 8).

The vertical offset between the two columns and lateral transport between them cause a lower position of the water table in hummocks compared to hollows generally equal to the specified different in height between them (0.3 m). There are slight differences in annual CH_4 flux between hummocks and hollows with consistent seasonal patterns between the two columns. A CH_4 pulse in the early growing season was simulated for both hummocks and hollows, with a slightly stronger pulse in hollows than hummocks. Temporal patterns of water table variations are similar for the two columns when there is no standing water in

hollows (WT < 0 for Hollow). When there is standing water in the hollow, there are substantial variations between the two columns due to horizontal flows and surface runoff from the hollows. Similar vertical patterns of DOC, acetate, and CH_4 concentrations occur for hummocks and hollows, with slightly higher concentrations in hummocks than in hollows. Meanwhile, there are apparent differences in CH_4, acetate and DOC concentration at the soil depth of ~0.3 m in hummocks versus hollows, which is consistent with the assumption of 0.3 m elevation difference in the surface of hummocks and hollows.

4. Discussion

4.1. Controls on CH_4 Flux and Transport Pathways

The ranking of all parameters responsible for CH_4 flux and transport using a sensitivity analysis can be used to indicate the most essential processes contributing to surface CH_4 fluxes and the most critical field measurements needed to better understand and predict CH_4 fluxes in response to environmental change. Simulated warming does change the relative importance of the parameters controlling CH_4 processes, indicating the critical impacts of warming on biogeochemical processes. Specifically with warming, the turnover rate of dissolved organic matter (*k_dom*) becomes a more sensitive parameter, indicating the need for observations of this quantity under the experimental treatments. The sensitivity of this parameter in addition to other parameters associated with acetoclastic methanogenesis indicate the importance of this process under environmental change.

The sensitivity analysis showed that the most important process for CH_4 dynamics in our model is acetoclastic methanogenesis, followed by the rate of acetate production, indicating that environmental factors controlling acetoclastic methanogenesis are likely the most important parameter(s) for the land-atmosphere CH_4 flux (Xu et al., 2015). For example, acetate porewater concentration, water content in the field controlling acetate production, and plant root exudation have been confirmed to be critical in affecting CH_4 flux (Conrad, 1989; Whiting & Chanton, 1993; Zona et al., 2009). The impacts of warming on the simulated fluxes will be discussed further in a subsequent manuscript.

The sensitivity analysis confirmed the importance of substrate production and microbial functional groups as two important determinants on CH_4 cycling, indicating substrate limitation in the peatland and microbial suppression. This is consistent with previous field studies for substrate limitation of CH_4 production (Hatala et al., 2012; McEwing et al., 2015). The substrate for CH_4 production may come from soil organic matter mineralization or vegetation root exudation. Further experiment and modeling traceability are needed to address this issue. Carbon dioxide and CH_4 isotopic capability in this model might be a useful solution to this issue, and it deserves future efforts.

The optimized version of the model generally produced accurate predictions of CH_4 fluxes. This result is consistent with the results of a previous SPRUCE modeling study (Ma et al., 2017). That study involved parameter optimization and sensitivity analysis using the TECO-SPRUCE model, which has reduced complexity of CH_4 and vegetation modules compared to ELM-SPRUCE. That study found a stronger influence of temperature sensitivity parameters on surface CH_4 fluxes, suggesting that model may be more responsive to experimental warming. Ma et al. (2017) also predicted a higher contribution of plant-mediated transport to CH_4 fluxes, suggesting that changes in vegetation composition may be more important in their model for predicting responses to warming treatments. These sensitivity analyses indicated that differences in model structure are likely contributing to a divergence in predictions despite calibration using pre-treatment observations. A companion paper to this study using ELM-SPRUCE to conduct warming simulations indeed indicates a muted warming response of CH_4 fluxes compared to the TECO study (Yuan et al., 2021). This highlights the need for additional studies at the site using multiple models. As a result, we have initiated a model intercomparison project for this purpose.

One specific concern for the ELM-SPRUCE predictions is the overestimation of modeled CH_4 flux compared with auto-chamber measurements of CH_4 flux in hummocks and hollows despite closer agreement with the other two measurement methods. This may be due in part to the experimental design. Specifically, in the auto-chamber experiments, aboveground vascular vegetation was clipped limiting plant-mediated transport and root exudation of labile DOM (Gill et al., 2017). Before clipping, the auto-chambers gave similar CH_4 fluxes to those measured by (Hanson et al., 2016). The reported CH_4 flux from auto-chamber

method is ~10%–30% lower than the flux obtained with large-collar approach and static chamber approach that capture a portion of the vegetation (Figure 4). In the future, model simulations could be designed to replicate this effect by performing simulations without the presence of specific vegetation types. Our study estimated that ebullition accounts for 23.5% of the CH_4 flux, which is much larger than the 1% estimated by Gill et al. (2017). The reason might be that small area (0.3 m diameter of the collar) in that study excluded open water, where ebullition usually occurs, and their approach only captures larger bubbles that were identified by non-linearities in CH_4 emissions. Other studies show that smaller bubbles may be an important source of ebullition (Prairie & del Giorgio, 2013). Overall our estimate falls in the range of 10–60% as reported by a large number of field experiments (Chanton et al., 1989; Mer & Roger, 2001; Tokida et al., 2007).

4.2. Key Features of the New Model

There are several key features of this new version of ELM-SPRUCE. First, the model integrates improvements in soil biogeochemistry and CH_4 dynamics described here with previous hydrologic improvements for two microtopography columns and parallel efforts to include a representation of moss. While previous modeling efforts have generally focused on specific components of wetland systems, these improvements allow for simulations with mechanistic representation of vegetation, hydrology, and soil biogeochemistry processes simultaneously, and this in turn can facilitate the examination of key feedbacks at the SPRUCE site. The vertically resolved representation of the model structure is critical for ecosystems with complex, depth-dependent belowground mechanisms, such as peatlands. In addition, the representation of site-specific plant functional types will allow exploration of how differences in productivity and mortality among these types may impact the site soil biogeochemistry under environmental change. For example, the recently observed decline in *Sphagnum* productivity (Norby et al., 2019) and shifts in the vascular plant community composition may have profound impacts on CH_4 cycling.

The highly mechanistic representation of biogeochemistry also allows model integration with the multiple types of observational data that are being collected as part of the SPRUCE experiment. For example, in this study, we compared the model output with observational data for CH_4 substrates, CH_4 concentration, and different transport pathways, in addition to the surface flux. This modeling approach provides a framework to understand how CH_4 dynamics respond to external environmental change. Meanwhile, this model is able to test the similar stimulation impacts of warming and elevated CO_2 on CH_4 flux with different mechanisms, which will be explored in future work. As the treatment data streams become available, we expect to simultaneously integrate this information with ELM-SPRUCE, continuously improving model performance and developing a mechanistic understanding of key processes and feedbacks contributing to carbon cycle responses. The model will also help to identify key processes, pools and temperature responses that experimentalists need to measure further to constrain key prediction uncertainties.

Importantly, ELM-SPRUCE allows us to determine if it is necessary to include this level of biogeochemical detail to successfully model the effects of warming and elevated CO_2 on CH_4 dynamics. The simpler TECO modeling framework has been a useful and highly successful testbed for an integrative approach, having been used to assimilate data on soil processes and snow (Huang et al., 2017), vegetation and soil carbon cycling (Jiang et al., 2018) and methane (Ma et al., 2017) in an ecological forecasting framework (Huang et al., 2019). ELM-SPRUCE, a considerably more complex and computationally demanding model, is currently being integrated into this forecasting framework using novel, efficient techniques for model-data integration (Lu et al., 2018). ELM-SPRUCE will allow additional valuable sources of data to be integrated into the model that are already being collected in the experimental enclosures, including vegetation productivity for specific functional types, DOM and acetate concentration profiles, CH_4 production profiles, measurements of microbial biomass, and partitioning of acetoclastic and hydrogenotrophic methanogenesis through isotopic analysis.

4.3. Importance of Model Timestep

The timestep of model output also affects the model performance in comparison with field observational data. This study showed that the hourly output is more consistent with observational CH_4 flux than the modeled daily CH_4 flux. We infer that the observational data tend to be highly variable with finer time steps,

which is consistent with the upscaling of ecosystem function. For example, the range of hourly flux in CH_4 is much wider than the daily flux (Figure 4). This is primarily caused by the large variation of temperature and precipitation at a sub-daily level. It is well known that the finer-scale ecosystem functions are more variable compared with coarse scale results (Hatala et al., 2012), and aggregating over space or time, if possible, may be necessary for comparison with models. It is important to conduct model evaluation at appropriate time scales to match the observational data, but also experimental designs should consider the appropriate time scale on which the ecosystem functions are measured and evaluated to maximize their relevance for modeling frameworks.

5. Conclusions and Future Directions

Here we extend the ELM-SPRUCE model (Griffiths et al., 2017; Shi et al., 2015) to include new capabilities for predicting CH_4 fluxes and variables associated with underlying production, oxidation, and transport mechanisms. ELM_SPRUCE is now an integrative site-scale model that simulates CH_4 dynamics from multiple perspectives including CH_4 substrate, CH_4 concentration in the soil profile, surface flux of CH_4, transport pathways, and microbial mechanisms driving the production and oxidation of CH_4. The model is used to predict pre-treatment conditions at the SPRUCE experiment site in a northern Minnesota peatland ecosystem. When model parameters are optimized using observations, the model accurately predicts the magnitude of and seasonal variations in CH_4 fluxes, as well as vertical profiles of DOC, acetate, and CH_4 within the peat layers. A parameter sensitivity analysis indicates that several parameters dominate uncertainties in CH_4 flux predictions including the turnover rate of dissolved organic matter, the maximum acetate production rate, and the growth rate of acetoclastic methanogens. Temperature sensitivity parameters are less important than indicated by previous studies. Our modeling framework, implemented within an Earth system model, lends itself naturally to regional and global scaling.

In the future, we expect improvements from ELM-SPRUCE to be fully integrated into the land component of the E3SM climate model. However, there are significant limitations in the current model structure and methods for spatial scaling that must be addressed to extend our model for regional and global relevance. Extending the ELM-SPRUCE model to account for variations in hydrology, vegetation, and sources of CH_4 fluxes over space and time is critical for eventual inclusion in an Earth system model. Variations in hydrology may strongly affect vegetation growth and peat decomposition with feedbacks on microtopography and peat properties, leading to different site microclimates and substrates for CH_4 processes (Waddington et al., 2015). Understanding how microtopography, hydrologic state variables and CH_4 fluxes are related is critical. Small differences in microtopography and developmental state can cause large differences in CH_4 emissions at seemingly similar sites, emphasizing the need for mechanistically based scaling techniques (Zalman et al., 2018). Microtopographic characteristics are currently observed with high accuracy at regular time intervals within the enclosures using terrestrial laser scanning (Graham et al., 2020), and this work could be extended over larger spatial scales, providing a key input for model-based scaling and parameterization of the Shi et al. (2015) hydrology module in ELM-SPRUCE over larger spatial scales. A spatially explicit version of ELM-SPRUCE must also have the ability to predict changes in vegetation productivity and community composition from warming and eCO_2 that likely feed back to CH_4 cycling. Ecosystem warming has already caused substantial changes to vegetation phenology at the SPRUCE site (Richardson et al., 2018), and changes in vegetation community composition may affect the ecosystem structure and function (Johnson et al., 2005), leading to different responses of CO_2 and CH_4 fluxes over long timescales (Ward et al., 2013). The introduction of dynamic vegetation into ELM-SPRUCE, for example, by integrating the Ecosystem Demography and CLM4.5 models (Fisher et al., 2015) is necessary to predict a realistic temporal evolution of vegetation across a range of sites. Finally, including isotopic tracers in our simulations is also necessary to trace the sources of the surface CH_4 flux and compare to observations across different sites. For example, homoacetogenesis is a key process for methanogenesis (Ye et al., 2014). At SPRUCE, it has been shown that this homoacetogenesis is an important process, that rates increase with temperature, and is important in the competition for H_2 with hydrogenotrophic methanogenesis (Leeways, 2019). An isotopic module will enhance our understanding of this process and its influence on surface CH_4 fluxes. ^{13}C and ^{14}C have already been incorporated in the current ELM version, but the isotopic module needs to be extended to

represent the effects CH_4 production and oxidation and other microbial processes (e.g., homoacetogenesis) on these isotopes.

A key goal of our ELM-SPRUCE modeling effort is eventual application to other wetland systems. A promising result for eventual spatial upscaling is that carbon cycle model simulations at wetland eddy covariance sites are fairly accurate in predicting gross and net carbon fluxes, especially when the models include realistic hydrology (Sulman et al., 2012). A mechanistic model-based upscaling will help integrate the observations obtained with site-level enclosure measurements with CO_2 and CH_4 fluxes measured to the larger footprints of eddy covariance towers over wetland sites. We can then assess the accuracy of these simulations across a variety of wetland tower sites, and better understand how key model sensitivities vary across sites using established methods (Ricciuto et al., 2018). Global simulations may then be performed using existing CH_4 modeling protocols (e.g., Melton et al., 2013). This will allow us to better understand the implications of the ambitious SPRUCE experiment for global peatlands, carbon cycling and terrestrial feedbacks to the climate system.

Data Availability Statement

Model code used in these simulations are available on the Github repository at http://doi.org/10.5281/zenodo.3733924. Model simulation output used in this analysis will be made publicly available on the SPRUCE project website https://mnspruce.ornl.gov and can be accessed at https://doi.org/10.25581/spruce.082/1638024.

Acknowledgments
This material is based upon work supported by the US Department of Energy, Office of Science, Office of Biological and Environmental Research. Oak Ridge National Laboratory is managed by UT-Battelle, LLC, for the US Department of Energy under contract DE-AC05-00OR22725. The views expressed in this article do not necessarily represent the views of the US Department of Energy or the United States Government. The authors would like to thank Randall K. Kolka, USDA Forest Service, Northern Research Station for working in collaboration with the Oak Ridge National Laboratory to enable access to and use of the S1-Bog of the Marcell Experimental Forest for the SPRUCE experiment and affiliated studies. This research used resources of the Compute and Data Environment for Science (CADES) at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

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