Running title: Microtopographic impacts on CO₂ and CH₄

Mechanistic Modeling of microtopographic impacts on CO₂ and CH₄ fluxes in an Alaskan tundra ecosystem using the CLM-Microbe model

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Abstract

Spatial heterogeneity in Arctic tundra is identified as a key control on CO$_2$ and CH$_4$ cycling, largely depending on changes in soil hydrological and thermal regimes, thereby vegetation and microbial communities. The CLM-Microbe model has been constructed to simulate microbial processes of CH$_4$ production and consumption: acetoclastic and hydrogenotrophic methanogenesis, aerobic and anaerobic methanotrophy. In this study we validated the CLM-Microbe against CO$_2$ and CH$_4$ fluxes measured by static chambers and an eddy covariance (EC) tower covering troughs, center, rim and transition features of low- and high-centered polygons (LCPs and HCPs) during 2012-2013 at Barrow, Alaska. Annual CH$_4$ emission was higher in troughs than center and rim of LCPs, which was reconstructed by the CLM-Microbe model. Modeled results showed that low elevated landscape types (troughs, transitions and LCP center) have larger CH$_4$ emission with greater seasonal variations than high elevated landscape types (rims and HCP center). Sensitivity analysis indicated that substrates (acetate, CO$_2$+H$_2$) availability for methanogenesis is the most important factor determining CH$_4$ emission in Arctic tundra ecosystems, and the amount of Rubisco enzyme and plant respiration largely affect the net ecosystem carbon exchange (NEE) and ecosystem respiration (ER). Modeled CH$_4$ flux for microtopographic features were upscaled to EC domain based on an area-weighted approach. Model underestimated the CH$_4$ emission within the EC domain by 20.1% and 25.0% at daily and hourly time steps, respectively. The CLM-Microbe has capability to simulate CO$_2$ and CH$_4$ fluxes for Arctic polygonal landscapes and therefore the microtopographic effects. This modeling study affirms the importance of spatial heterogeneity on simulating and projecting CO$_2$ and CH$_4$ fluxes across the Arctic landscapes.
Keywords: Arctic Tundra, CH₄ flux, Microtopographic, Sensitivity Analysis, Net Carbon Exchange
1. Introduction

Arctic tundra soils store a large amount of carbon (C) and have long been considered as a sink for CO₂ while it might be alternated by the recent climate warming [Oechel et al., 1994]. Meanwhile, the Arctic soils were considered as either a net sink [Jørgensen et al., 2015; Oh et al., 2016], or a net source of atmospheric CH₄ [Lau et al., 2015; Nauta et al., 2015; Tan et al., 2015]. Spatial heterogeneity in Arctic tundra is the key source for large variability and uncertainty in methane (CH₄) emission and ecosystem C exchange [Xu et al., 2014]. One primary feature of Arctic tundra is the polygonal ground pattern due to the annual freeze-thaw cycles [Throckmorton et al., 2015; Davidson et al., 2016], creating a complex mosaic of wetting and drying microtopographic features that greatly alter soil water contents and active layer depths [Grant et al., 2017], soil pH and O₂ availability [Zona et al., 2011; Lipson et al., 2012], thermal conductivity and soil temperature [Kumar et al., 2016], vegetation types [Davidson et al., 2016] and height [von Fischer et al., 2010], nutrient availability [Semenchuk et al., 2015]. Changes in these abiotic and biotic factors lead to substantial impacts on the spatial and temporal variations in CH₄ and CO₂ fluxes in the Arctic.

CH₄ dynamics in Arctic tundra is mainly determined by the balance between CH₄ production in anaerobic condition and CH₄ consumption in aerobic condition of soils [von Fischer et al., 2010; Xu et al., 2015]. The O₂ diffusion is restricted by the excessive surface water in low elevated grounds, leading to anoxic condition for anaerobic methanogenesis [Lipson et al., 2012]. Anoxic soils potentially contain a large amount of organic C and deep organic layer thickness, influence the alternative electron acceptors availability such as iron and humic substances, further regulate CH₄ production rate [Miller et al., 2015]. Great aeration in the well-drained high elevated
grounds stimulates CH₄ oxidation by methanotrophs [Nazaries et al., 2013]. CH₄ transport through diffusion and ebullition depending on hydration dynamics also differ among the microtopographic features [Ebrahimi and Or, 2017]. Soil thermal conductivity is affected by soil water saturation, which links greater active layer depth to saturated soils [Atchley et al., 2016]. Thicker active layer and saturated conditions in low elevated ground lead to a more rapid CH₄ emission [Grant et al., 2017].

Vegetation type and height are recognized as the good predictors for CH₄ emission from Arctic soils. Taller and vascular plants with extensive root systems across the heterogeneous landscapes favor the plant-mediated transport of CH₄ to atmosphere [von Fischer et al., 2010; Davidson et al., 2016]. Moreover, high plant biomass is normally resulted from high gross primary productivity (GPP), resulting in high soil C input that can provides abundant substrates for methanogenesis. Net ecosystem exchange of CO₂ (NEE) and ecosystem respiration (ER), as the two components of GPP [Davidson et al., 2016], are also influenced by the heterogeneous microtopography in Arctic tundra. Increased water table strongly lowers ecosystem respiration (ER) by reducing soil oxygen availability [Olivas et al., 2010]. ER is highly sensible to soil water table, which can shortly be doubled in drying tundra [Olivas et al., 2010]. NEE can be suppressed by decreased soil water table, because the increase in photosynthesis is lower than that in root and microbial activity [Olivas et al., 2010]. Microtopographic effects on CO₂ fluxes largely depend on the responses of photosynthesis and ecosystem respiration to soil water conditions [Zona et al., 2011; Grant et al., 2017].
In order to more accurately capture the fine-scale variations in CH$_4$ and CO$_2$ fluxes in Arctic tundra, microtopographic effects need to be considered by ecosystem models as microbial functions such as fermentation, C mineralization, methanogenesis and methanotrophy differ among the wet and dry polygons [Taş et al., 2018]. Many process-based CH$_4$ models have incorporated the mechanisms of CH$_4$ production, consumption and transport pathways into their frameworks, such as the ecosys model [Grant et al., 2017], CLM-Microbe [Xu et al., 2015], CLM4Me [Riley et al., 2011], LPJ-WHyMe [Wania et al., 2010], and NEST-DNDC [Zhang et al., 2012]. Several CH$_4$ models have been developed and applied for permafrost regions to investigate the mechanisms of microtopography effecting on temporal and spatial variations of CH$_4$ flux in Arctic tundra [Grant et al., 2017; Kaiser et al., 2017]. The ecosys model indicated that microtopography determines CO$_2$ and CH$_4$ emission by regulating soil water content, active layer depth and O$_2$ availability [Grant et al., 2017]. The CLM-Microbe model defines 15 soil layers and 25 plant functional types (PFTs) and simulates microbial functional groups for methanogenesis and methanotrophy [Xu et al., 2015], therefore, potentially has the capability to capture small-scale variations of CH$_4$ production and consumption affected by microtopography in Arctic tundra. The CLM-Microbe model was validated for simulating CH$_4$ emission from incubation experiments of Arctic soils with constant soil temperature and water content [Xu et al., 2015]. However, it has not been tested for observational CH$_4$ fluxes with respect to microtopographic landscape types in Arctic tundra.

In this study, we simulated the microtopographic impacts on CH$_4$ and CO$_2$ fluxes using the CLM-Microbe model at the Barrow Environmental Observatory (BEO) near Barrow, Alaska, as part of the Department of Energy’s Next-Generation Ecosystem Experiment (NGEE) Arctic...
Sampling area C (100 m × 100 m) was chosen and two primary topographic types in Area C are low-centered polygons (LCPs) and high-centered polygons (HCPs) with the internal features of centers, rims, transitions and troughs. We conducted the model simulations for seven landscape types, including troughs, LCP center, LCP rim, LCP transition, HCP center, HCP rim, and HCP transition. To evaluate the modeled plot-level CH₄ fluxes for upscaling to an eddy covariance (EC) domain, we utilized the area-weighted method for estimations of EC fluxes.

2. Methodology

2.1. Site Information and Experimental Data

2.1.1. Site Description

Our study area is located within the Barrow Environmental Observatory (BEO), ~6 km east of Barrow, Alaska (71.3 N, 156.5 W), as part of the U.S. Department of Energy’s Office of Science Next Generation Ecosystem Experiments (NGEE) Arctic project (https://ngee-arctic.ornl.gov/). The landscapes are highly heterogeneous with polygonal ground patterns. Barrow has a polar maritime climate with mean annual air temperature of −12.0 and 3.3 °C and during winter and summer (June–August), and with mean annual precipitation of 173 mm and the majority of precipitation falling during summer months [Liljedahl et al., 2011]. Snowmelt usually ends in early to mid-June and the wind direction is predominantly from east to west throughout the year [Wainwright et al., 2017]. The dominant plants are mosses (Dicranum elongatum, Sphagnum), lichens and vascular plants (such as Carex aquatilis); plant distribution is governed by surface moisture variability [Zona et al., 2011].

[Insert Figure 1 here]
The NGEE-Arctic project has established four 100 m ×100 m intensively-sampled areas within the BEO (Figure 1). Area C was chosen for model simulations according to the available dataset of landscape classification. The landscape classification map for Area C was produced based on the surface elevation generated by the NGEE-Arctic project (Figure 2). Seven landscape types were differentiated within the study area: troughs (35.0% of total area), LCP center (6.9%), LCP rim (12.2%), LCP transition (14.3%), HCP center (13.2%), HCP rim (12.2%), and HCP transition (6.2%) (Figure 2). Characteristics of soil profiles and difference in surface elevations for all the landscape types showed in Figure 2. Rims of LCPs and HCPs had the highest soil organic matter density but smallest percentage of plant functional types (PFTs) on the natural vegetation land unit (Table 1). Troughs have the lowest soil organic matter density, while LCP center and LCP transition have a majority of the PFTs (Table 1).

2.1.2. Data Availability

The plot-level CH₄ and CO₂ fluxes from static closed chambers were observed on several dates during July to September of 2012-2013 (available at http://ngee-arctic.ornl.gov/). In 2013, the transparent and opaque surface chambers were placed for troughs, LCP center and LCP rim. CO₂ flux from the transparent chambers was considered as the net ecosystem exchange (NEE), while that from opaque chambers as ecosystem respiration (ER). In the study area, an eddy covariance (EC) tower was installed, and CH₄ and NEE fluxes were measured at a half-hourly time step during May-September of 2013, which are available from the NGEE Arctic project. Daily and
hourly fluxes of CH\textsubscript{4} and CO\textsubscript{2} fluxes were calculated based on the half-hourly EC data. Detailed information about measurement protocols is posted in the NGEE Arctic archives (http://ngee-arctic.ornl.gov/).

2.2. Model Experiment

2.2.1. Model Description and Driving Forces

The CLM-Microbe model branched from the framework of default CLM 4.5 by developing a new representation of CH\textsubscript{4} production and consumption [Xu et al, 2015], in association with the decomposition subroutines in CLM4.5 [Thornton and Rosenbloom, 2005; Thornton et al., 2007]. It developed new mechanisms of dissolved organic carbon fermentation, hydrogenotrophic methanogenesis, acetoclastic methanogenesis, aerobic methanotrophy, anaerobic methanotrophy, and H\textsubscript{2} production based on the known processes (Thauer et al., 1989; 2008), and adopted from previous modeling studies [Grant, 1998; Segers, 1998; Walter and Heimann, 2000; Kettunen, 2003; Zhuang et al., 2004; Tian et al., 2010; Riley et al., 2011] (Figure 1). Detailed information of the CLM-Microbe is available in Xu et al. (2015). In this paper, we modified the hydrological processes for each micro-topographic type to mimic the actual environmental conditions. For lower elevated features, troughs, LCP center, HCP center, LCP transition, HCP transition are poorly drained and their soil water tables are usually above the surface ground in summer that creating the inundated and anoxic conditions, we changed the parameters for soil water content (h2osoi_vol) to be 1.0 in module of mkarbinitMod.F90, surface runoff (qflx_surf) to be 0 in module of SoilHydrologyMod.F90, and the inundated fraction (finundated) to be 0.99 in module of microbeMod.F90. For well-drained higher elevation features of LCP rim, HCP center and HCP rim, the parameters for surface runoff and inundated fraction were kept unchanged, and soil
water contents were reduced to be 0.3. Detailed mathematical expressions for CH$_4$ production and consumption, and microbial growth and death were organized in Xu et al. (2015), and the other improved features including bacteria and fungi in the CLM-Microbe model which is available at https://github.com/email-clm/clm-microbe. The version used in this study was checked out on June 18, 2018.

The meteorological data includes shortwave and longwave radiations, air temperature, relative humidity, wind speed, and precipitation from 1 January 1991 to 31 December 2014 derived by Xu and Yuan (2016) from the Barrow, AK, station of NOAA/Earth System Laboratory, Global Monitoring Division (http://www.esrl.noaa.gov/gmd/obop/brw/). The other soil property data is from the global dataset. The meteorological data is gap-filled and at a 1/2-hour time step.

2.2.2 Model Implementation

To simulate the plot-level CH$_4$ flux for different micro-topographic types, the model implementation was carried out with three stages, following the default CLM4.5. Firstly, the accelerated model spin-up was set up for 2000 years to allow the system accumulate C. Then a final spin-up for 50 years allows the modeled system to reach a relatively steady state. After the final spin-up, the transient model simulation was set up to cover 1850-2014.

The model parameterization started with the default parameters in Xu et al. (2015). To get a good fit for observed CH$_4$ and CO$_2$ fluxes for each microtopographic type, model parameterization was performed to determine the optimal values of parameters related to microbial processes, plant growth and ecosystem respiration. We primarily focused on the parameters for substrate
supply for methanogenesis (e.g. acetic acid), plant growth and maintenance respiration, C
distribution to different pools and microbial structure based on the extant knowledge of micro-
topographic impacts on C cycling in Arctic tundra. The transient simulations of 1850-2014 were
operated at daily and hourly time steps for model validation with observational data from static
chambers and the EC tower. Linear regression with no interception was conducted to evaluate
modeled CH$_4$, NEE and ER fluxes comparing with observed data from chambers for troughs,
LCP center and LCP rim. The error statistics were used to distinguish the difference between
modeled and observed fluxes, including $R^2$ on the platform of R Studio (version 1.1.456).

2.2.3. Area-weighted Upscaling

To test if the modeled CH$_4$ fluxes are qualified for upscaling, we used the area-weighted method
to upscale the modeled plot-level CH$_4$ and CO$_2$ fluxes to the EC domain. Due to the limitation of
landscape classification data, the EC domain was confined into an area of 100 m $\times$ 100 m. The
area-weighted method includes the information of landscape heterogeneity in the upscaling
process. The up-scaled flux was calculated by the following equation:

$$F = \sum_{i=1}^{n} f_i \times Area_i$$

where $F$ is the up-scaled plot flux for the entire study area, $f_i$ is the plot-level CH$_4$ or CO$_2$ fluxes
for a given landscape type on a given time period, $Area_i$ is the fraction of each major landscape
type within the EC domain [Davison et al., 2016]. The data qualification was tested by the error
statistics of $R^2$. 

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2.2.4 Sensitivity Analysis

To identify the most important process and most sensitive parameters for CH\textsubscript{4} and CO\textsubscript{2} dynamics in Arctic tundra, a global sensitivity analysis was conducted for each microtopographic type, and it focused on 15 parameters related to plant and microbial processes (Table 2). For each parameter, we set up model simulations with +20% and -20% to compare the responses in modeled CH\textsubscript{4} and CO\textsubscript{2} fluxes for 2013. The index \( S \) comparing the change in model output relative to model response for a nominal set of parameters was calculated based on the equation [Xu 2010; Xu et al., 2015]:

\[
S = \frac{(R_a - R_n) / R_n}{(P_a - P_n) / P_n}
\] (2),

where \( S \) is the ratio of the standardized change in model response to the standardized change in parameter values. \( R_a \) and \( R_n \) are model responses for altered and nominal parameters, respectively, and \( P_a \) and \( P_n \) are the altered and nominal parameters, respectively. \( S \) is negative if the direction of model response opposes the direction of parameter change [Xu et al., 2015].

[Insert Table 2 here]

3. Results

3.1 Model Performance against CH\textsubscript{4} and CO\textsubscript{2} Fluxes across the Arctic Landscape

Types

In the summer of 2012-2013, larger CH\textsubscript{4} emission with high variations was observed in troughs than that in LCP center and LCP rim, and the CLM-Microbe model was capable to simulate the differences in CH\textsubscript{4} dynamics among three landscape types (Figure 3a-c). Overall, modeled CH\textsubscript{4} fluxes were more consistent with observed data for troughs \((R^2 = 0.7111, p < 0.0001)\) and LCP center \((R^2 = 0.2820, p = 0.0507)\) than LCP rim (Table 3). CH\textsubscript{4} flux for LCP rim was
underestimated by 49.8\% during 2012-2013 ($R^2 = 0.2075, p = 0.0435$), primarily due to a great discrepancy in 2012 (Table 3). During the total study period, the model performed better for CH$_4$ fluxes in 2013 for the three landscape types (Figure 3).

![Insert Figure 3 here]

![Insert Figure 4 here]

![Insert Table 3 here]

NEE is determined by the difference between ER and GPP. The model captured the changes of NEE during the summer of 2013 (Figure 3d-f), with consistency for troughs ($R^2 = 0.9569, p = 0.0007$) and LCP center ($R^2 = 0.9194, p = 0.0025$), respectively (Table 3). However, NEE was obviously underestimated in LCP rim (Figure 4f). In 2013, ER was overestimated by 47.3\% for trough ($R^2 = 0.8316, p < 0.0001$), 39.2\% for LCP center ($R^2 = 0.9188, p < 0.0001$) and 64.5\% for LCP rim ($R^2 = 0.88, p < 0.0001$), respectively (Table 3).

3.2 Variability and Seasonality of CH$_4$ and CO$_2$ Fluxes across the Arctic Landscape

Types

Modeled CH$_4$ and CO$_2$ fluxes exhibited large variabilities among seven landscape types. In warm seasons, low elevated landscape types of troughs, LCP center, LCP transition and HCP transition showed larger CH$_4$ emission and C uptake with greater variations than higher elevated landscape types of LCP rim, HCP rim and HCP center (Figure 5). Among all the landscape types, greater CH$_4$ emission was associated with higher GPP and higher absolute values of NEE (Figure 5). ER and HR were roughly higher in HCP center while lower in troughs and LCP center during the whole growing seasons (Figure 5).
Great seasonal variations in CH$_4$ dynamics were modeled across the landscape types. At the beginning of spring, all the types showed a burst release of CH$_4$ flux, corresponding to the early spring thaw. During the growing seasons, troughs and LCP transition had similar seasonality of CH$_4$ and NEE fluxes and showed the highest CH$_4$ fluxes and lowest NEE in the summer (Figure 5). High elevated landscape types of LCP rim and HCP rim tended to have smaller variations during the growing seasons. A rapid increase of CH$_4$ emission was modeled in the middle of growing seasons for HCP transition, and a sudden rise of NEE, ER and HR were modeled for troughs, LCP transition, LCP center and HCP center during the late of growing seasons (Figure 5).

### 3.3 Annual Budget of CH$_4$ and CO$_2$ Fluxes across the Landscape Types

Annual CH$_4$ fluxes were estimated for all seven landscape types with an average of 2.4 g C m$^{-2}$ y$^{-1}$ in a range of 0.7 to 4.0 g C m$^{-2}$ (Table 5). The largest annual CH$_4$ emission rate in HCP transition was 6.1 times of the smallest CH$_4$ emission in LCP rim. Troughs and transitions of LCPs and HCPs contributed a large proportion of CH$_4$ emission in Arctic regions. According to their areal fractions, HCPs and LCPs have estimated to have annual CH$_4$ fluxes of 2.1 and 2.2 g C m$^{-2}$ y$^{-1}$, respectively, which were smaller than that in troughs of 3.6 g C m$^{-2}$ y$^{-1}$. In the year of 2013, most of the landscape types were considered as the net source of C, except troughs. In 2013, 21.1 g C m$^{-2}$ y$^{-1}$ of C can be fixed in troughs (Table 5). The average of NEE across the landscapes was 104.3 g C m$^{-2}$ y$^{-1}$, of 77.7% from HCPs and 25.2% from LCPs. The range of annual ER estimates was from 582.7 to 928.0 g C m$^{-2}$ y$^{-1}$ for all landscape types with an average
of 716.8 g C m\(^{-2}\) y\(^{-1}\). HCP center had the largest ER while troughs had the smallest for the whole year. Troughs, LCP center and LCP rim with smaller NEE estimates were also estimated to have smaller ER budget.

3.4 Upscaling CH\(_4\) and NEE Fluxes

Modeled CH\(_4\) and NEE fluxes from all seven landscape types were up-scaled to the EC domain of our study area based on the fraction of each landscape type; we found a high consistency between the up-scaled CO\(_2\) and CH\(_4\) flux and the observations from the EC tower (Figure 6, 7). A correlation analysis showed that better estimations of CH\(_4\) and NEE fluxes for the entire EC domain were at a daily time step than that at an hourly time step (Figure 7). CH\(_4\) fluxes were underestimated both at daily (\(R^2 = 0.7931, p < 0.0001\)) and hourly (\(R^2 = 0.6135, p < 0.0001\)) time steps, while NEE was underestimated at daily time step (\(R^2 = 0.2843, p < 0.0001\)) but overestimated at hourly time step (\(R^2 = 0.3464, p < 0.0001\)) (Table 5). Annual CH\(_4\) fluxes was also calculated for the EC domain, which was 2.8 g C m\(^{-2}\) y\(^{-1}\) higher than the arithmetic average of estimates for all the landscape types. The entire study area has been estimated to release C at a rate of 73.8 g C m\(^{-2}\) y\(^{-1}\) in 2013, and it has emitted 692.9 g C m\(^{-2}\) y\(^{-1}\) via the processes of ecosystem respiration.
3.5. Sensitivity Analysis

CH$_4$ and CO$_2$ fluxes were sensible at different degrees to the 15 parameters related to available carbon mineralization, CH$_4$ production, growth of methanogens, decomposition, photosynthesis, growth and maintenance respiration. CH$_4$ fluxes were strongly sensible to the parameters of AceProdAcemax and ACMinQ10, followed by YAceMethanogens, GrowRAceMethanogens, KAce and $k_{dom}$ for all landscape types (Figure 8a), which indicated that acetic acid production and available carbon mineralization were the key controls on CH$_4$ dynamics in Arctic ecosystems. Growth of methanogens also regulated CH$_4$ fluxes by effects on CH$_4$ production, and changes of decomposition rate of dissolved organic matter had a positive influence on CH$_4$ fluxes for all the landscapes except LCP rim (Figure 8a). In high elevated features of LCP rim, HCP rim and HCP center, CH$_4$ emission was affected by Rubisco enzyme functioning in photosynthesis. In HCP rim, CH$_4$ dynamics also responded to changes in decomposition rate of fungi biomass and growth respiration (Figure 8a). Growth and maintenance respiration and Rubisco enzyme were also the components of altering CH$_4$ fluxes in low elevated features but exhibiting opposite directions of effects (Figure 8a).

[Insert Figure 8 here]

The most important processes of CO$_2$ dynamics were related to photosynthesis and respiration that controlling C uptake and release among the Arctic landscapes. The fraction of leaf nitrogen (N) in Rubisco enzyme was identified as the primary factor on NEE and ER (Figure 8b, 8c). Increased amount of Rubisco enzyme led to a rise of NEE in troughs, LCP rim and HCP rim, but a reduce of NEE for LCP center, LCP transition, HCP transition and HCP center, and a significant decrease in ER for all landscapes (Figure 8b, 8c). For high elevated grounds of LCP
rim, HCP rim and HCP center, NEE dynamics showed negative responses to $ACMinQ10$ and positive response to $AceProdACmax$, which showed that acetic acid production was also important for C uptake from atmosphere (Figure 8b). In troughs, responses of NEE were sensible to many other parameters related to acetic acid production, decomposition and respiration (Figure 8b). Beside the parameter for Rubisco enzyme, ER dynamics was affected by maintenance respiration in high elevated features, as well as in low elevated troughs and LCP center (Figure 8c). Additionally, variations in decomposition rate of bacteria and fungi biomass in LCP center could result in changes of ER (Figure 8c).

4. Discussions

4.1. Microtopographic Impacts on $CH_4$ and $CO_2$ Fluxes

Microtopography determines $CH_4$ and $CO_2$ dynamics in Arctic polygonal tundra through affecting the hydrological and thermal processes, thereby soil water content, active layer depth, vegetation and microbial functional groups in ecosystem carbon exchange [Zona et al., 2011; Lipson et al., 2012; Davidson et al., 2016; Grant et al., 2017]. Ice wedges in the Arctic Coastal Plain uplift the terrain, creating a complex mosaic of microtopographic features with poorly-drained low-centered polygons surrounding by high rims and well-drained high-centered polygons surrounding by low troughs. Soil water contents were higher in the low elevated troughs, LCP transition, LCP center and HCP transition than high elevated LCP rim, HCP rim and HCP center, which explained the great variations of $CH_4$ emissions in Arctic ecosystems [Grant et al., 2017]. Larger $CH_4$ emission was observed and modeled in troughs associated with its higher soil water content, creating the anaerobic condition for methanogens acting on $CH_4$.
production. Due to the similar hydrological conditions, high CH$_4$ fluxes were modeled in LCP center, LCP transition and HCP transition.

CH$_4$ flux is strictly produced by methanogens at very low O$_2$ concentration in soils, mainly converted from acetic acid and CO$_2$+H$_2$. Substrate supply for methanogenesis affected by acetic acid production and decomposition of dissolved organic matter were recognized as the key constraints for CH$_4$ dynamics in Arctic polygonal landscapes. During growing seasons, absolute values of NEE reflect how much net C uptake from atmosphere via ecosystem productivity and determine the amount of C input as litters. Low elevated features with larger C uptake would provide abundant substrates for microbial decomposition, thereby facilitate CH$_4$ production by methanogens. In high elevated rims and HCP center, CH$_4$ emission was sensible to the Rubisco enzyme functioning in plant photosynthesis, partly because the great plant biomass resulted from high efficiency of photosynthesis led to a rise in the plant-mediated transport of CH$_4$ from soil to atmosphere.

Microtopographic effects on CO$_2$ dynamics were also led by the changes in movement of soil water and snowmelt, as well as O$_2$ availability. Plants tends to grow better in low elevated troughs with high soil water content, but aerobic respiration was suppressed by the low dissolved O$_2$ concentration in saturated soils. Greater ER in high elevated ground were modeled in agreement with previous studies [Zona et al., 2011]. HCP center emitted the largest emission of CO$_2$ and troughs had the lowest CO$_2$ emission during growing seasons, largely caused by the difference in soil O$_2$ availability for heterotrophic respiration. Obviously, ER showed a strong negative response to the amount of Rubisco enzyme across the Arctic landscapes. NEE dynamics
was regulated by a combination of photosynthesis and respiration that produced substantial uncertainties in NEE across Arctic landscape. Most landscape models do not consider the microtopographic effects in simulating C fluxes. It might cause large biases; therefore, better modeling microtopographic impacts on soil thermal dynamic, hydrology, and further biogeochemistry is critical for model application to C cycling in the Arctic.

4.2. Model Performance at Different Time Steps

The biological processes occur at second scale, which is inconsistent with the field measurement. While the ecosystem function is more important at hourly, daily, and month, and annual scale, and the CLM-Microbe performance at hourly, daily, and annual time scale. The model performance against observational data is more consistent with observational data at daily time scale, indicating the model was not doing well in capturing some spark fluxes at hourly scale. The “CH₄ outbreak” in spring season has been widely recognized in recent decades [Song et al, 2012], that how to better simulate the outbreak events is an important topic for ecosystem modeling community.

Up-scaled CH₄ and NEE fluxes based on the CLM-Microbe model were able to capture most variations of measured EC fluxes at both daily and hourly time steps. In the EC domain, dynamics of CH₄ and NEE at daily time step was modeled more accurately comparing with simulations for hourly CH₄ and NEE fluxes. This is probably because the key factors or processes of CH₄ and CO₂ dynamics could be slightly different across the temporal scales, but they are well-defined with stable priorities in the model according to the extant knowledge usually from observations at long time scales.
4.3. Model Implication

This study provides three implications to model developments and scientific understanding of the C dynamic in the Arctic. Firstly, the CLM-Microbe performed well in capturing the variabilities in CH₄ and CO₂ fluxes among primary polygonal landscapes in Arctic tundra, which emphasize the importance of spatial heterogeneity in simulating CO₂ and CH₄ fluxes and should be well-represented in ecosystem models. Model simulated that the troughs and transitions have estimated to release CH₄ fluxes of 3.6 ~ 4.0 g C m⁻² y⁻¹ annually, while rims had a smaller annual CH₄ emission of 0.7 ~ 1.1 g C m⁻² y⁻¹. Differences in annual estimations were likely due to the saturated and anoxic conditions in low elevational areas that promote anaerobic methanogenesis, leading to a higher CH₄ emission. The annual CH₄ estimate of 2.7 g C m⁻² y⁻¹ for the entire study area was low compared with values reported for similar ecosystems in Arctic tundra [Reeburgh et al., 1998; Wille et al., 2008]. The discrepancy might be explained by the low organic matter density or small proportions of PFTs in our study area; for example, the small PFTs coverage shrinks the plant-mediated transport of CH₄ to the atmosphere that lowers CH₄ emission [Bhullar et al., 2013]. CH₄ emission was recognized to have large responses to acetate production and available carbon mineralization as substrate supply for methanogenesis largely relies on the decomposition of soil organic matter [Kim, 2015].

Second, the potential shifts in Arctic tundra ecosystem as C sink or source is valuable information for climate projection. This study showed that troughs are the only net CO₂ sink among all landscape types and play an important role in ecosystem C storage due to its high areal fraction of 35% in the entire study area. Despite the strongest influence of Rubisco enzyme on
NEE and ER, dynamics of net C exchange in troughs were also sensitive to many processes related to C mineralization and distribution among the soil C pools. It suggests that troughs would rapidly shift to a net C source even with a small-scale change in C cycling in response to global warming. Annual estimations indicated that HCPs had a higher strength of CO$_2$ source than LCPs, which was 310% higher than LCPs. Additionally, greater ER was estimated in HCPs than LCPs, and HCP center had the greatest ER of 928.0 g C m$^{-2}$ comparing with other landscape types. Since LCPs may eventually subside into HCPs, CO$_2$ emission from Arctic soils tends to increase fast not only because of effects of climate changes but also changes in landscape patterns.

Last but not the least, this study advocates the mechanistic modeling of C cycling to better estimate CO$_2$ and CH$_4$ fluxes across the Arctic tundra ecosystem. It is well known that differences in CH$_4$ and CO$_2$ emission across the Arctic landscapes are directly led by the mechanisms and dynamics of microbial activities in relation to C mineralization, decomposition, respiration, methanogenesis, and methanotrophy. By inclusions of these microbial processes, the CLM-Microbe model allows us to understand the mechanisms of Arctic C cycling according to the production and consumption processes of CO$_2$ and CH$_4$. Soil dissolved organic carbon (DOC), CH$_4$ and CO$_2$ concentrations were modeled and compared with the measured concentrations regarding the landscape types and soil depths for few data points [Yang et al., 2013] (Table S1). Modeled DOC concentrations were ~1.6 times the measurements at the middle layer of soils in troughs on DOY 183 and DOY 240 of 2013, which suggested that the model could be useful for simulating the soil chemical concentrations. In Arctic ecosystems, large CH$_4$ emission in saturated soils was modeled with great CH$_4$ production using acetic acids, which was
consistent with the large amount of modeled acetoclastic methanogens. CH$_4$ oxidation was strengthened by high O$_2$ availability in top soils of rims and HCP center comparing with the saturated troughs and transitions. Moreover, differences of CH$_4$ transport via diffusion, ebullition and the plant-mediated transport were modeled with seasonal variations. Large CH$_4$ fluxes emitted from soils were associated with fast plant growing during summer. Furthermore, soil microbial structure and biomass can be considered to understand the CO$_2$ and CH$_4$ dynamics, by model simulations for microbial biomass C and N of bacteria, fungi, acetoclastic and hydrogenotrophic methanogens, aerobic and anaerobic methanotrophs.

4.4. The Way forwards

The CLM-Microbe model is able to simulate the microbial processes for belowground carbon cycling and surface CO$_2$ and CH$_4$ flux. Although compromising results proved the robustness of the CLM-Microbe model in simulating surface CO$_2$ and CH$_4$ fluxes, a number of tasks are identified as follow-up to this study. First, although the upscaling results with area-weighted approach seems compromising, the dominant roles of landscape types weakened the variations in C flux. An upscaling with mechanistic model should provide more accurate quantification of the C flux at regional scale, as well as higher resolution C flux at both spatial and temporal scales. Second, belowground C dynamics, for example, dissolved organic carbon, acetate, CO$_2$ and CH$_4$ concentrations, are important variables and precursors for observed surface gas fluxes. We call for a data-model integration approach to better integrate the observational data and better simulate belowground processes and surface flux. Third, the hydrological dynamics is the key controls to biogeochemical processes particular under the changing Arctic and the dramatic impact of climate on hydrology. Improving the model’s ability to better simulate hydrology is an
important endeavor for simulating soil biogeochemistry. Fourth, the microbial genomic information is the most accurate information for microbial functions, yet it has not been well utilized for model parameterization. The CLM-Microbe model is capable to simulate relative abundance of methanogenesis; thus, it is worthwhile to improve the model to better simulate the microbial functional groups responsible for CH$_4$ production and consumption. Fifth, although the C flux data, particularly the CH$_4$ flux, has been in shortage across the Arctic tundra ecosystem, recent projects and technical improvement have allowed year-round measurements. Those data would be a good constrain for the CLM-Microbe model at multiple scales, therefore, a multiscale “MODEX” framework to better integrate multiple sources of observational data to quantify gas flux and understand their underlay mechanisms in the Arctic is needed, it should benefit the scientific community.

5. Conclusions

This study reported the applications of the CLM-Microbe model to seven microtopographic landscape types in the Arctic tundra, Barrow, AK. The model results were promising with a consistency with observational gas fluxes. Modeled results showed that low elevated landscape types (troughs, transitions and LCP center) have larger CH$_4$ emission with greater seasonal variations than high elevational landscape types (rims and HCP center), which was caused by the higher soil saturation in the low elevated landscape types. Model sensitivity analysis showed that substrate (acetate, CO$_2$+H$_2$) availability for methanogens was the most important factor that determining CH$_4$ emission in Arctic ecosystems, and plant photosynthesis largely affected the NEE and ER. The model performed better for simulating the daily EC fluxes than hourly fluxes, that indicates the importance of time scale on simulating gas fluxes.
The CLM-Microbe model has been successfully applied to CO$_2$ and CH$_4$ fluxes in the several major Arctic landscape type at the plot level. Given the large spatial heterogeneity across the Arctic tundra ecosystem, it is more appropriate to conduct a mechanistic model-based upscaling to estimate the ecosystem-atmosphere exchange of CH$_4$ and CO$_2$ to the EC tower and further to the Pan-Arctic.
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Figure Caption

**Figure 1.** The landscape classification map for Area C (100 m × 100 m). Red indicates high surface elevation and blue indicates low surface elevation (Yuan et al., 2017).

**Figure 2.** Information of soil profiles and topography in study area (Yuan et al., 2017).

**Figure 3.** Modeled (a-c) CH₄ fluxes, (d-f) net ecosystem carbon exchange (NEE) and (g-i) ecosystem respiration (ER) for troughs (blue lines), LCP center (red lines) and LCPrim (green lines) comparing with observed fluxes from static chambers (purple points with error bars) from May to September in 2012 and 2013. Observed fluxes from Torn (2016).

**Figure 4.** Scatter plots of observed vs modeled (a-c) CH₄ fluxes, (d-f) net ecosystem carbon exchange (NEE), and (g-i) ecosystem respiration (ER) for troughs (blue points), LCP center (red points) and LCPrim (green points), with linear lines of best fit (no interception) and 95% confidence interval for regression line shaded grey.

**Figure 5.** Modeled (a) CH₄ fluxes, (b) net ecosystem carbon exchange (NEE), (c) ecosystem respiration (ER), (d) gross primary production (GPP) and (e) heterotrophic respiration (HR) for all seven landscapes types in 2013.

**Figure 6.** Upscaled (a, b) CH₄ fluxes and (c, d) net ecosystem carbon exchange (NEE) comparing with measured fluxes from an eddy covariance (EC) tower centered in the study area at the daily (a, c) and hourly (b, d) time steps in 2013. Lines indicate the upscaled fluxes and purple points indicate measured fluxes.

**Figure 7.** Scatter plots of measured vs upscaled CH₄ (a, b) and net ecosystem carbon exchange (NEE) (c, d) at daily (a, c) and hourly (b, d) time steps for the eddy covariance (EC) domain of study area in 2013, with linear lines of best fit (no interception) and 95% confidence interval for regression line shaded grey.

**Figure 8.** Sensitivity analysis for model response of (a) CH₄ fluxes, (b) net ecosystem carbon exchange (NEE) and (c) ecosystem respiration (ER) to 15 parameters (KAce, ACMiQ10, AceProdACmax, H2ProdAcemax, KH2ProdAce, KCO2ProdAce, KCO2ProdCH₄, GrowRAceMethanogens, YAceMethanogens, k_dom, k_bacteria, k_fungi, flnr, grperc, br_mr) for troughs (tg), LCP transition (lt), LCP center (lc), HCP transition (ht), LCP rim (lr), HCP rim (hr) and HCP center (hc). “+” and “-” indicate 20% increase or 20% decrease of parameter values. Dark red and darker blue indicate a stronger positive or negative model response to parameter change. S is negative if the direction of model response opposes the direction of parameter change.
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Figure 2. Diagram depicting the several landscape types and their soil properties along vertical profiles within study area (Yuan et al., 2017)
Figure 3. Modeled (a-c) CH$_4$ fluxes, (d-f) net ecosystem carbon exchange (NEE) and (g-i) ecosystem respiration (ER) for troughs (blue lines), LCP center (red lines) and LCP rim (green lines) comparing with observed fluxes from static chambers (purple points with error bars) from May to September in 2012 and 2013. Observed fluxes from Torn (2016).
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Table 1. Soil organic matter and percent plant functional types (PFTs) on the natural vegetation land unit for all seven landscape types

| Sites           | Organic matter density (kg m⁻³) | Percent PFTs (%) |
|-----------------|---------------------------------|------------------|
| Troughs         | 14.2                            | 7.4              |
| LCP center      | 38.0                            | 59.7             |
| LCP rim         | 125.0                           | 6.5              |
| LCP transition  | 26.1                            | 59.7             |
| HCP center      | 88.4                            | 19.7             |
| HCP rim         | 125.0                           | 6.5              |
| HCP transition  | 113.5                           | 19.7             |
Table 2. Key parameters for sensitivity analysis

| Parameters               | Ecological meanings                                                                 |
|--------------------------|--------------------------------------------------------------------------------------|
| K_Ace                    | Half-saturation coefficient of available carbon mineralization                       |
| A_CminQ10                | Temperature sensitivity of available carbon mineralization                           |
| AoceneProdAcmax          | Maximum rate of acetic acid production from available carbon                          |
| H2ProdAcecmax            | Maximum rate of $H_2$ production from available acetic acid                          |
| K_H2ProdAce              | Half-saturation coefficient of conversion of $H_2$ and $CO_2$ to acetic acid         |
| K_CO2ProdAce             | Assuming it is half of that for $H_2$ based on stoichiometry theory                 |
| K_CO2ProdCH4             | Half coefficient of $CO_2$ for methane production from $H_2$                         |
| GrowRAceMethanogens      | Growth rate of acetoclastic methanogens                                              |
| Y_AceMethanogens         | Growth efficiency of acetoclastic methanogens                                         |
| k_dom                    | Decomposition rate constant dissolved organic matter                                 |
| k_bacteria               | Decomposition rate constant biomass of bacteria                                      |
| k_fungi                  | Decomposition rate constant biomass of fungi                                        |
| flnr                     | Fraction of leaf N in the Rubisco enzyme                                             |
| grperc                   | Growth respiration parameter                                                         |
| br_mr                    | Base rate of maintenance respiration                                                |
Table 3. Linear regression analysis for CH₄ fluxes, net ecosystem carbon exchange (NEE) and ecosystem respiration (ER) modeled and observed from static chambers for troughs, LCP center and LCP rim in 2012 and 2013

| Variables | Sites          | Estimate | Std. Error | t value | Pr(>|t|) | R²     |
|-----------|----------------|----------|------------|---------|---------|--------|
| CH₄ (2012) | Troughs       | 1.0008   | 0.1504     | 6.6556  | 0.0000* | 0.7111 |
|           | LCP center    | 1.0167   | 0.4683     | 2.1708  | 0.0507* | 0.2820 |
|           | LCP rim       | 0.5023   | 0.2314     | 2.1710  | 0.0435* | 0.2075 |
| CH₄ (2012) | Troughs       | 0.7188   | 0.2604     | 2.7606  | 0.0398* | 0.6038 |
|           | LCP center    | NA       | NA         | NA      | NA      | NA     |
|           | LCP rim       | 0.2986   | 0.2630     | 1.1352  | 0.3077  | 0.2049 |
| CH₄ (2013) | Troughs       | 1.0626   | 0.1827     | 5.8153  | 0.0001* | 0.7381 |
|           | LCP center    | 1.0167   | 0.4683     | 2.1708  | 0.0507* | 0.2820 |
|           | LCP rim       | 1.0925   | 0.4363     | 2.5040  | 0.0277* | 0.3432 |
| NEE (2013) | Troughs       | 0.9961   | 0.1057     | 9.4236  | 0.0007* | 0.9569 |
|           | LCP center    | 1.0572   | 0.1565     | 6.7567  | 0.0025* | 0.9194 |
|           | LCP rim       | 0.2160   | 0.2339     | 0.9235  | 0.4080  | 0.1757 |
| ER (2013)  | Troughs       | 1.4729   | 0.1913     | 7.6977  | 0.0000* | 0.8316 |
|           | LCP center    | 1.3922   | 0.1195     | 11.6504 | 0.0000* | 0.9188 |
|           | LCP rim       | 1.6449   | 0.1753     | 9.3829  | 0.0000* | 0.8800 |

Note: “*” indicate the significant level < 0.1.
Table 4. Estimation of annual budgets for CH₄ fluxes, net ecosystem carbon exchange (NEE) and ecosystem respiration (ER) for all seven landscape types and the EC domain based on modeled daily fluxes in 2013

| Sites         | CH₄ (gC m⁻² yr⁻¹) | NEE (gC m⁻² yr⁻¹) | ER (gC m⁻² yr⁻¹) |
|---------------|------------------|------------------|------------------|
| Troughs       | 3.6324           | -21.0825         | 582.7146         |
| LCPcenter     | 1.1454           | 3.0555           | 598.5198         |
| LCPrim        | 0.6555           | 19.5785          | 617.6598         |
| LCPtransition | 3.8352           | 160.9284         | 754.9855         |
| HCPcenter     | 2.3838           | 137.9404         | 927.9807         |
| HCPrim        | 1.0752           | 180.2766         | 776.3092         |
| HCPtransition | 3.9741           | 248.2191         | 759.4632         |
| EC domain     | 2.6710           | 73.8247          | 692.8553         |
Table 5. Linear regression analysis for CH$_4$ fluxes and net ecosystem carbon exchange (NEE) modeled and measured from the eddy covariance (EC) tower at daily and hourly time steps.

| Variables | Time step | Estimate | Std. Error | t value | Pr(>|t|) | $R^2$ |
|-----------|-----------|----------|------------|---------|---------|-------|
| CH$_4$    | Daily     | 0.7992   | 0.0440     | 18.1566 | 0.0000* | 0.7931 |
|           | Hourly    | 0.7505   | 0.0204     | 36.8406 | 0.0000* | 0.6135 |
| NEE       | Daily     | 0.7856   | 0.1242     | 6.3271  | 0.0000* | 0.2943 |
|           | Hourly    | 1.3001   | 0.0546     | 23.8009 | 0.0000* | 0.3464 |

Note: “*” indicate the significant level $< 0.1.$
Table S1. The comparison between modeled and observational belowground DOC, CO$_2$, and CH$_4$ concentrations (gC m$^{-3}$)

| DOY | Sites | Sample depth (cm) | Soil layer (CLM-Microbe) | DOC modeled | DOC observed | CO$_2$ modeled | CO$_2$ observed | CH$_4$ modeled | CH$_4$ observed |
|-----|-------|------------------|--------------------------|-------------|--------------|---------------|----------------|----------------|----------------|
| 183 | Center | 26 | 5 | 1419.74 | 30.60 | 0.00 | NA | 0.04 | NA |
| 240 | Center | 49 | 6 | 1422.88 | 1015.32 | 13.33 | NA | 0.28 | NA |
| 606 | Center | 10 | 4 | 1674.68 | 25.68 | 0.00 | NA | 0.02 | NA |
| 183 | Trough | 28 | 6 | 448.11 | 282.84 | 16.08 | 156.60 | 0.55 | 0.11 |
| 240 | Trough | 22 | 5 | 478.20 | 283.92 | 0.00 | 33.00 | 0.08 | 0.14 |
| 240 | Trough | 29 | 6 | 458.43 | 222.84 | 16.15 | NA | 0.59 | NA |
| 606 | Trough | 20 | 5 | 483.29 | 118.08 | 0.00 | 48.84 | 0.01 | 0.50 |
| 606 | Trough | 37 | 6 | 462.32 | 184.80 | 16.25 | 35.16 | 0.57 | 2.06 |
| 183 | Rim | 29 | 6 | 1064.58 | NA | 4.13 | NA | 0.09 | NA |
| 183 | Rim | 7 | 3 | 1120.60 | 29.16 | 618.30 | NA | 0.05 | NA |
| 240 | Rim | 7 | 3 | 1178.37 | 30.72 | 618.34 | NA | 0.14 | NA |
| 240 | Rim | 37 | 6 | 1073.85 | 66.72 | 4.20 | NA | 0.20 | NA |