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2	Running title: Microtopographic impacts on CO <sub>2</sub> and CH <sub>4</sub>
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5	Mechanistic Modeling of microtopographic impacts on CO <sub>2</sub> and CH <sub>4</sub> fluxes in
6	an Alaskan tundra ecosystem using the CLM-Microbe model
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#### 38 Abstract

39 Spatial heterogeneity in Arctic tundra is identified as a key control on CO<sub>2</sub> and CH<sub>4</sub> cycling, 40 largely depending on changes in soil hydrological and thermal regimes, thereby vegetation and 41 microbial communities. The CLM-Microbe model has been constructed to simulate microbial 42 processes of CH<sub>4</sub> production and consumption: acetoclastic and hydrogenotrophic 43 methanogenesis, aerobic and anaerobic methanotrophy. In this study we validated the CLM-44 Microbe against CO<sub>2</sub> and CH<sub>4</sub> fluxes measured by static chambers and an eddy covariance (EC) 45 tower covering troughs, center, rim and transition features of low- and high-centered polygons 46 (LCPs and HCPs) during 2012-2013 at Barrow, Alaska. Annual CH<sub>4</sub> emission was higher in 47 troughs than center and rim of LCPs, which was reconstructed by the CLM-Microbe model. 48 Modeled results showed that low elevated landscape types (troughs, transitions and LCP center) 49 have larger CH<sub>4</sub> emission with greater seasonal variations than high elevated landscape types 50 (rims and HCP center). Sensitivity analysis indicated that substrates (acetate,  $CO_2+H_2$ ) 51 availability for methanogenesis is the most important factor determining CH<sub>4</sub> emission in Arctic 52 tundra ecosystems, and the amount of Rubisco enzyme and plant respiration largely affect the net 53 ecosystem carbon exchange (NEE) and ecosystem respiration (ER). Modeled CH<sub>4</sub> flux for microtopographic features were upscaled to EC domain based on an area-weighted approach. 54 55 Model underestimated the CH<sub>4</sub> emission within the EC domain by 20.1% and 25.0% at daily and 56 hourly time steps, respectively. The CLM-Microbe has capability to simulate CO<sub>2</sub> and CH<sub>4</sub> 57 fluxes for Arctic polygonal landscapes and therefore the microtopographic effects. This 58 modeling study affirms the importance of spatial heterogeneity on simulating and projecting CO<sub>2</sub> 59 and CH<sub>4</sub> fluxes across the Arctic landscapes.

- 60 Keywords: Arctic Tundra, CH4 flux, Microtopographic, Sensitivity Analysis, Net Carbon
- 61 Exchange

### 62 **1.Introduction**

63

64 for CO<sub>2</sub> while it might be alternated by the recent climate warming [Oechel et al., 1994]. 65 Meanwhile, the Arctic soils were considered as either a net sink [Jørgensen et al., 2015; Oh et 66 al., 2016], or a net source of atmospheric CH<sub>4</sub> [Lau et al., 2015; Nauta et al., 2015; Tan et al., 67 2015]. Spatial heterogeneity in Arctic tundra is the key source for large variability and 68 uncertainty in methane (CH<sub>4</sub>) emission and ecosystem C exchange [Xu et al., 2014]. One 69 primary feature of Arctic tundra is the polygonal ground pattern due to the annual freeze-thaw 70 cycles [Throckmorton et al., 2015; Davidson et al., 2016], creating a complex mosaic of wetting 71 and drying microtopographic features that greatly alter soil water contents and active layer 72 depths [Grant et al., 2017], soil pH and O<sub>2</sub> availability [Zona et al., 2011; Lipson et al., 2012], 73 thermal conductivity and soil temperature [Kumar et al., 2016], vegetation types [Davidson et 74 al., 2016] and height [von Fischer et al., 2010], nutrient availability [Semenchuk et al., 2015].

Arctic tundra soils store a large amount of carbon (C) and have long been considered as a sink

Changes in these abiotic and biotic factors lead to substantial impacts on the spatial and temporal
 variations in CH<sub>4</sub> and CO<sub>2</sub> fluxes in the Arctic.

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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 O<sub>2</sub> 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 CH<sub>4</sub> oxidation by methanotrophs [*Nazaries et al., 2013*]. CH<sub>4</sub> 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 CH<sub>4</sub>
emission [*Grant et al., 2017*].

91

92 Vegetation type and height are recognized as the good predictors for CH<sub>4</sub> emission from Arctic 93 soils. Taller and vascular plants with extensive root systems across the heterogeneous landscapes 94 favor the plant-mediated transport of CH<sub>4</sub> to atmosphere [von Fischer et al., 2010; Davidson et 95 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 96 97 methanegenesis. Net ecosystem exchange of CO<sub>2</sub> (NEE) and ecosystem respiration (ER), as the 98 two components of GPP [Davidson et al., 2016], are also influenced by the heterogeneous 99 microtopography in Arctic tundra. Increased water table strongly lowers ecosystem respiration 100 (ER) by reducing soil oxygen availability [Olivas et al., 2010]. ER is highly sensible to soil 101 water table, which can shortly be doubled in drying tundra [Olivas et al., 2010]. NEE can be 102 suppressed by decreased soil water table, because the increase in photosynthesis is lower than 103 that in root and microbial activity [Olivas et al., 2010]. Microtopographic effects on CO<sub>2</sub> fluxes 104 largely depend on the responses of photosynthesis and ecosystem respiration to soil water 105 conditions [Zona et al., 2011; Grant et al., 2017].

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107 In order to more accurately capture the fine-scale variations in CH<sub>4</sub> and CO<sub>2</sub> fluxes in Arctic 108 tundra, microtopographic effects need to be considered by ecosystem models as microbial 109 functions such as fermentation, C mineralization, methanogenesis and methanotrophy differ 110 among the wet and dry polygons [*Tas et al., 2018*]. Many process-based CH<sub>4</sub> models have 111 incorporated the mechanisms of CH<sub>4</sub> production, consumption and transport pathways into their 112 frameworks, such as the ecosys model [Grant et al., 2017], CLM-Microbe [Xu et al., 2015], 113 CLM4Me [Riley et al., 2011], LPJ-WHyMe [Wania et al., 2010], and NEST-DNDC [Zhang et 114  $al_{...}$  2012]. Several CH<sub>4</sub> models have been developed and applied for permafrost regions to 115 investigate the mechanisms of microtopography effecting on temporal and spatial variations of 116 CH4 flux in Arctic tundra [Grant et al., 2017; Kaiser et al., 2017]. The ecosys model indicated 117 that microtopography determines CO<sub>2</sub> and CH<sub>4</sub> emission by regulating soil water content, active 118 layer depth and O<sub>2</sub> availability [Grant et al., 2017]. The CLM-Microbe model defines 15 soil 119 layers and 25 plant functional types (PFTs) and simulates microbial functional groups for 120 methanogenesis and methanotrophy [Xu et al., 2015], therefore, potentially has the capability to 121 capture small-scale variations of CH<sub>4</sub> production and consumption affected by microtopography 122 in Arctic tundra. The CLM-Microbe model was validated for simulating CH<sub>4</sub> emission from 123 incubation experiments of Arctic soils with constant soil temperature and water content [Xu et 124 al., 2015]. However, it has not been tested for observational CH<sub>4</sub> fluxes with respect to 125 microtopographic landscape types in Arctic tundra. 126

127 In this study, we simulated the microtopographic impacts on CH<sub>4</sub> and CO<sub>2</sub> fluxes using the

128 CLM-Microbe model at the Barrow Environmental Observatory (BEO) near Barrow, Alaska, as

129 part of the Department of Energy's Next-Generation Ecosystem Experiment (NGEE) Arctic

130	project. Sampling area C (100 m $\times$ 100 m) was chosen and two primary topographic types in
131	Area C are low-centered polygons (LCPs) and high-centered polygons (HCPs) with the internal
132	features of centers, rims, transitions and troughs. We conducted the model simulations for seven
133	landscape types, including troughs, LCP center, LCP rim, LCP transition, HCP center, HCP rim,
134	and HCP transition. To evaluate the modeled plot-level CH4 fluxes for upscaling to an eddy
135	covariance (EC) domain, we utilized the area-weighted method for estimations of EC fluxes.

# 137 2. Methodology

# 138 2.1. Site Information and Experimental Data

# 139 <u>2.1.1. Site Description</u>

140 Our study area is located within the Barrow Environmental Observatory (BEO), ~6 km east of 141 Barrow, Alaska (71.3 N, 156.5 W), as part of the U.S. Department of Energy's Office of Science 142 Next Generation Ecosystem Experiments (NGEE) Arctic project (https://ngee-arctic.ornl.gov/). 143 The landscapes are highly heterogeneous with polygonal ground patterns. Barrow has a polar 144 maritime climate with mean annual air temperature of -12.0 and 3.3 °C and during winter and 145 summer (June–August), and with mean annual precipitation of 173 mm and the majority of 146 precipitation falling during summer months [Liljedahl et al., 2011]. Snowmelt usually ends in 147 early to mid-June and the wind direction is predominantly from east to west throughout the year 148 [Wainwright et al., 2017]. The dominant plants are mosses (Dicranum elongatum, Sphagnum), 149 lichens and vascular plants (such as *Carex aquatilis*); plant distribution is governed by surface 150 moisture variability [Zona et al., 2011].

151

# [Insert Figure 1 here]

153

154	The NGEE-Arctic project has established four 100 m ×100 m intensively-sampled areas within
155	the BEO (Figure 1). Area C was chosen for model simulations according to the available dataset
156	of landscape classification. The landscape classification map for Area C was produced based on
157	the surface elevation generated by the NGEE-Arctic project (Figure 2). Seven landscape types
158	were differentiated within the study area: troughs (35.0% of total area), LCP center (6.9%), LCP
159	rim (12.2%), LCP transition (14.3%), HCP center (13.2%), HCP rim (12.2%), and HCP
160	transition (6.2%) (Figure 2). Characteristics of soil profiles and difference in surface elevations
161	for all the landscape types showed in Figure 2. Rims of LCPs and HCPs had the highest soil
162	organic matter density but smallest percentage of plant functional types (PFTs) on the natural
163	vegetation land unit (Table 1). Troughs have the lowest soil organic matter density, while LCP
164	center and LCP transition have a majority of the PFTs (Table 1).
165	[Insert Table 1 here]
166	
167	2.1.2. Data Availability
168	The plot-level CH <sub>4</sub> and CO <sub>2</sub> fluxes from static closed chambers were observed on several dates
169	during July to September of 2012-2013 (available at http://ngee-arctic.ornl.gov/). In 2013, the
170	transparent and opaque surface chambers were placed for troughs, LCP center and LCP rim. CO2
171	flux from the transparent chambers was considered as the net ecosystem exchange (NEE), while
172	that from opaque chambers as ecosystem respiration (ER). In the study area, an eddy covariance
173	(EC) tower was installed, and CH <sub>4</sub> and NEE fluxes were measured at a half-hourly time step
174	during May-September of 2013, which are available from the NGEE Arctic project. Daily and

hourly fluxes of CH<sub>4</sub> and CO<sub>2</sub> fluxes were calculated based on the half-hourly EC data. Detailed
information about measurement protocols is posted in the NGEE Arctic archives (http://ngeearctic.ornl.gov/).

178

#### 179 2.2. Model Experiment

## 180 <u>2.2.1. Model Description and Driving Forces</u>

181 The CLM-Microbe model branched from the framework of default CLM 4.5 by developing a 182 new representation of CH<sub>4</sub> production and consumption [Xu et al, 2015], in association with the 183 decomposition subroutines in CLM4.5 [Thornton and Rosenbloom, 2005; Thornton et al., 2007]. 184 It developed new mechanisms of dissolved organic carbon fermentation, hydrogenotrophic 185 methanogenesis, acetoclastic methanogenesis, aerobic methanotrophy, anaerobic methanotrophy, 186 and H<sub>2</sub> production based on the known processes (Thauer et al., 1989; 2008), and adopted from 187 previous modeling studies [Grant, 1998; Segers, 1998; Walter and Heimann, 2000; Kettunen, 188 2003; Zhuang et al., 2004; Tian et al., 2010; Riley et al., 2011] (Figure 1). Detailed information 189 of the CLM-Microbe is available in Xu et al. (2015). In this paper, we modified the hydrological 190 processes for each micro-topographic type to mimic the actual environmental conditions. For 191 lower elevated features, troughs, LCP center, HCP center, LCP transition, HCP transition are 192 poorly drained and their soil water tables are usually above the surface ground in summer that 193 creating the inundated and anoxic conditions, we changed the parameters for soil water content 194 (h2osoi vol) to be 1.0 in module of mkarbinitMod.F90, surface runoff (qflx surf) to be 0 in 195 module of SoilHydrologyMod.F90, and the inundated fraction (finundated) to be 0.99 in module 196 of microbeMod.F90. For well-drained higher elevation features of LCP rim, HCP center and 197 HCP rim, the parameters for surface runoff and inundated fraction were kept unchanged, and soil

199	and consumption, and microbial growth and death were organized in Xu et al. (2015), and the
200	other improved features including bacteria and fungi in the CLM-Microbe model which is
201	available at https://github.com/email-clm/clm-microbe. The version used in this study was
202	checked out on June 18, 2018.
203	
204	The meteorological data includes shortwave and longwave radiations, air temperature, relative
205	humidity, wind speed, and precipitation from 1 January 1991 to 31 December 2014 derived by
206	Xu and Yuan (2016) from the Barrow, AK, station of NOAA/Earth System Laboratory, Global
207	Monitoring Division (http://www.esrl. noaa.gov/gmd/obop/brw/). The other soil property data is
208	from the global dataset. The meteorological data is gap-filled and at a 1/2-hour time step.
209	
210	2.2.2 Model Implementation
211	To simulate the plot-level CH4 flux for different micro-topographic types, the model
212	implementation was carried out with three stages, following the default CLM4.5. Firstly, the
213	accelerated model spin-up was set up for 2000 years to allow the system accumulate C. Then a
214	final spin-up for 50 years allows the modeled system to reach a relatively steady state. After the
215	final spin-up, the transient model simulation was set up to cover 1850-2014.
216	
217	The model parameterization started with the default parameters in Xu et al. (2015). To get a good
218	fit for observed CH <sub>4</sub> and CO <sub>2</sub> fluxes for each microtopographic type, model parameterization
219	was performed to determine the optimal values of parameters related to microbial processes,
220	plant growth and ecosystem respiration. We primarily focused on the parameters for substrate

water contents were reduced to be 0.3. Detailed mathematical expressions for  $CH_4$  production

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221 supply for methanogenesis (e.g. acetic acid), plant growth and maintenance respiration, C 222 distribution to different pools and microbial structure based on the extant knowledge of micro-223 topographic impacts on C cycling in Arctic tundra. The transient simulations of 1850-2014 were 224 operated at daily and hourly time steps for model validation with observational data from static 225 chambers and the EC tower. Linear regression with no interception was conducted to evaluate 226 modeled CH<sub>4</sub>, NEE and ER fluxes comparing with observed data from chambers for troughs, 227 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). 228

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## 230 <u>2.2.3. Area-weighted Upscaling</u>

To test if the modeled CH<sub>4</sub> fluxes are qualified for upscaling, we used the area-weighted method to upscale the modeled plot-level CH<sub>4</sub> and CO<sub>2</sub> 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<sub>4</sub> or CO<sub>2</sub> fluxes for a given landscape type on a given time period, *Area<sub>i</sub>* 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  $R^2$ .

242 <u>2.2.4 Sensitivity Analysis</u>

To identify the most important process and most sensitive parameters for  $CH_4$  and  $CO_2$  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  $CH_4$  and  $CO_2$  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  $[Xu \ 2010; Xu \ et \ al., \ 2015]$ :

250 
$$S = \frac{(Ra-Rn)/Rn}{(Pa-Pn)/Pn} \quad (2),$$

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].

- 255 [Insert Table 2 here]
- 256
- 257 **3. Results**

## 258 3.1 Model Performance against CH<sub>4</sub> and CO<sub>2</sub> Fluxes across the Arctic Landscape

259 *Types* 

```
260 In the summer of 2012-2013, larger CH<sub>4</sub> emission with high variations was observed in troughs
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- than that in LCP center and LCP rim, and the CLM-Microbe model was capable to simulate the
- 262 differences in CH<sub>4</sub> dynamics among three landscape types (Figure 3a-c). Overall, modeled CH<sub>4</sub>
- fluxes were more consistent with observed data for troughs ( $R^2 = 0.7111$ , p < 0.0001) and LCP
- 264 center ( $R^2 = 0.2820$ , p = 0.0507) than LCP rim (Table 3). CH<sub>4</sub> flux for LCP rim was

265	underestimated by 49.8% during 2012-2013 ( $R^2 = 0.2075$ , $p = 0.0435$ ), primarily due to a great
266	discrepancy in 2012 (Table 3). During the total study period, the model performed better for CH <sub>4</sub>
267	fluxes in 2013 for the three landscape types (Figure 3).
268	[Insert Figure 3 here]
269	[Insert Figure 4 here]
270	[Insert Table 3 here]
271	
272	NEE is determined by the difference between ER and GPP. The model captured the changes of
273	NEE during the summer of 2013 (Figure 3d-f), with consistency for troughs ( $R^2 = 0.9569$ , $p =$
274	0.0007) and LCP center ( $R^2 = 0.9194$ , $p = 0.0025$ ), respectively (Table 3). However, NEE was
275	obviously underestimated in LCP rim (Figure 4f). In 2013, ER was overestimated by 47.3% for
276	trough ( $R^2 = 0.8316$ , $p < 0.0001$ ), 39.2% for LCP center ( $R^2 = 0.9188$ , $p < 0.0001$ ) and 64.5% for
277	LCP rim ( $R^2 = 0.88$ , $p < 0.0001$ ), respectively (Table 3).
278	
279	3.2 Variability and Seasonality of CH4 and CO2 Fluxes across the Arctic Landscape
280	Types
281	Modeled CH <sub>4</sub> and CO <sub>2</sub> fluxes exhibited large variabilities among seven landscape types. In warm
282	seasons, low elevated landscape types of troughs, LCP center, LCP transition and HCP transition
283	showed larger CH <sub>4</sub> emission and C uptake with greater variations than higher elevated landscape
284	types of LCP rim, HCP rim and HCP center (Figure 5). Among all the landscape types, greater
285	CH <sub>4</sub> emission was associated with higher GPP and higher absolute values of NEE (Figure 5). ER
286	and HR were roughly higher in HCP center while lower in troughs and LCP center during the
287	whole growing seasons (Figure 5).

290	Great seasonal variations in CH <sub>4</sub> dynamics were modeled across the landscape types. At the
291	beginning of spring, all the types showed a burst release of CH4 flux, corresponding to the early
292	spring thaw. During the growing seasons, troughs and LCP transition had similar seasonality of
293	CH4 and NEE fluxes and showed the highest CH4 fluxes and lowest NEE in the summer (Figure
294	5). High elevated landscape types of LCP rim and HCP rim tended to have smaller variations
295	during the growing seasons. A rapid increase of CH <sub>4</sub> emission was modeled in the middle of
296	growing seasons for HCP transition, and a sudden rise of NEE, ER and HR were modeled for
297	troughs, LCP transition, LCP center and HCP center during the late of growing seasons (Figure
298	5).

299

# 300 3.3 Annual Budget of CH<sub>4</sub> and CO<sub>2</sub> Fluxes across the Landscape Types

Annual CH<sub>4</sub> fluxes were estimated for all seven landscape types with an average of 2.4 g C m<sup>-2</sup> y<sup>-</sup> 301  $^1$  in a range of 0.7 to 4.0 g C m  $^2$  (Table 5). The largest annual CH4 emission rate in HCP 302 transition was 6.1 times of the smallest CH4 emission in LCP rim. Troughs and transitions of 303 304 LCPs and HCPs contributed a large proportion of CH<sub>4</sub> emission in Arctic regions. According to 305 their areal fractions, HCPs and LCPs have estimated to have annual CH<sub>4</sub> fluxes of 2.1 and 2.2 g C m<sup>-2</sup> y<sup>-1</sup>, respectively, which were smaller than that in troughs of 3.6 g C m<sup>-2</sup> y<sup>-1</sup>. In the year of 306 307 2013, most of the landscape types were considered as the net source of C, except troughs. In 2013, 21.1 g C m<sup>-2</sup> y<sup>-1</sup> of C can be fixed in toughs (Table 5). The average of NEE across the 308 landscapes was 104.3 g C m<sup>-2</sup> y<sup>-1</sup>, of 77.7% from HCPs and 25.2% from LCPs. The range of 309 annual ER estimates was from 582.7 to 928.0 g C m<sup>-2</sup> y<sup>-1</sup> for all landscape types with an average 310

of 716.8 g C m<sup>-2</sup> y<sup>-1</sup>. HCP center had the largest ER while troughs had the smallest for the whole 311 312 year. Troughs, LCP center and LCP rim with smaller NEE estimates were also estimated to have 313 smaller ER budget.

314

#### [Insert Table 4 here]

- 315
- 3.4 Upscaling CH<sub>4</sub> and NEE Fluxes 316

317 Modeled CH<sub>4</sub> and NEE fluxes from all seven landscape types were up-scaled to the EC domain 318 of our study area based on the fraction of each landscape type; we found a high consistency 319 between the up-scaled CO<sub>2</sub> and CH<sub>4</sub> flux and the observations from the EC tower (Figure 6, 7). 320 A correlation analysis showed that better estimations of CH<sub>4</sub> and NEE fluxes for the entire EC 321 domain were at a daily time step than that at an hourly time step (Figure 7). CH<sub>4</sub> fluxes were underestimated both at daily ( $R^2 = 0.7931$ , p < 0.0001) and hourly ( $R^2 = 0.6135$ , p < 0.0001) time 322 steps, while NEE was underestimated at daily time step ( $R^2 = 0.2843$ , p < 0.0001) but 323 overestimated at hourly time step ( $R^2 = 0.3464$ , p < 0.0001) (Table 5). Annual CH<sub>4</sub> fluxes was 324 also calculated for the EC domain, which was 2.8 g C m<sup>-2</sup> y<sup>-1</sup> higher than the arithmetic average 325 of estimates for all the landscape types. The entire study area has been estimated to release C at a 326 rate of 73.8 g C m<sup>-2</sup> y<sup>-1</sup> in 2013, and it has emitted 692.9 g C m<sup>-2</sup>y<sup>-1</sup> via the processes of 327 328 ecosystem respiration.

- 329
- [Insert Table 5 here] [Insert Figure 6 here] 330
- 331 [Insert Figure 7 here]
- 332

#### 333 **3.5.** Sensitivity Analysis

334

335 carbon mineralization, CH<sub>4</sub> production, growth of methanogens, decomposition, photosynthesis, 336 growth and maintenance respiration. CH<sub>4</sub> fluxes were strongly sensible to the parameters of 337 AceProdAcemax and ACMinQ10, followed by YAceMethanogens, GrowRAceMethanogens, 338 *KAce* and *k dom* for all landscape types (Figure 8a), which indicated that acetic acid production 339 and available carbon mineralization were the key controls on CH<sub>4</sub> dynamics in Arctic 340 ecosystems. Growth of methanogens also regulated CH<sub>4</sub> fluxes by effects on CH<sub>4</sub> production, 341 and changes of decomposition rate of dissolved organic matter had a positive influence on CH4 fluxes for all the landscapes except LCP rim (Figure 8a). In high elevated features of LCP rim, 342 343 HCP rim and HCP center, CH<sub>4</sub> emission was affected by Rubisco enzyme functioning in 344 photosynthesis. In HCP rim, CH<sub>4</sub> dynamics also responded to changes in decomposition rate of 345 fungi biomass and growth respiration (Figure 8a). Growth and maintenance respiration and 346 Rubisco enzyme were also the components of altering CH<sub>4</sub> fluxes in low elevated features but 347 exhibiting opposite directions of effects (Figure 8a).

CH<sub>4</sub> and CO<sub>2</sub> fluxes were sensible at different degrees to the 15 parameters related to available

348

#### [Insert Figure 8 here]

349

The most important processes of CO<sub>2</sub> 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

356 rim, HCP rim and HCP center, NEE dynamics showed negative responses to ACMinQ10 and 357 positive response to AceProdACmax, which showed that acetic acid production was also 358 important for C uptake from atmosphere (Figure 8b). In troughs, responses of NEE were sensible 359 to many other parameters related to acetic acid production, decomposition and respiration 360 (Figure 8b). Beside the parameter for Rubisco enzyme, ER dynamics was affected by 361 maintenance respiration in high elevated features, as well as in low elevated troughs and LCP 362 center (Figure 8c). Additionally, variations in decomposition rate of bacteria and fungi biomass 363 in LCP center could result in changes of ER (Figure 8c).

364

# 365 **4. Discussions**

# 366 4.1. Microtopographic Impacts on CH<sub>4</sub> and CO<sub>2</sub> Fluxes

367 Microtopography determines CH<sub>4</sub> and CO<sub>2</sub> dynamics in Arctic polygonal tundra through 368 affecting the hydrological and thermal processes, thereby soil water content, active layer depth, 369 vegetation and microbial functional groups in ecosystem carbon exchange [Zona et al., 2011; 370 Lipson et al., 2012; Davidson et al., 2016; Grant et al., 2017]. Ice wedges in the Arctic Coastal 371 Plain uplift the terrain, creating a complex mosaic of microtopographic features with poorly-372 drained low-centered polygons surrounding by high rims and well-drained high-centered 373 polygons surrounding by low troughs. Soil water contents were higher in the low elevated 374 troughs, LCP transition, LCP center and HCP transition than high elevated LCP rim, HCP rim 375 and HCP center, which explained the great variations of CH<sub>4</sub> emissions in Arctic ecosystems 376 [Grant et al., 2017]. Larger CH4 emission was observed and modeled in troughs associated with 377 its higher soil water content, creating the anaerobic condition for methanogens acting on CH4

production. Due to the similar hydrological conditions, high CH<sub>4</sub> fluxes were modeled in LCP
center, LCP transition and HCP transition.

380

381  $CH_4$  flux is strictly produced by methanogens at very low  $O_2$  concentration in soils, mainly 382 converted from acetic acid and CO<sub>2</sub>+H<sub>2</sub>. Substrate supply for methanogenesis affected by acetic 383 acid production and decomposition of dissolved organic matter were recognized as the key 384 constraints for CH<sub>4</sub> dynamics in Arctic polygonal landscapes. During growing seasons, absolute 385 values of NEE reflect how much net C uptake from atmosphere via ecosystem productivity and 386 determine the amount of C input as litters. Low elevated features with larger C uptake would 387 provide abundant substrates for microbial decomposition, thereby facilitate CH<sub>4</sub> production by 388 methanogens. In high elevated rims and HCP center, CH<sub>4</sub> emission was sensible to the Rubisco 389 enzyme functioning in plant photosynthesis, partly because the great plant biomass resulted from 390 high efficiency of photosynthesis led to a rise in the plant-mediated transport of CH<sub>4</sub> from soil to 391 atmosphere.

392

393 Microtopographic effects on  $CO_2$  dynamics were also led by the changes in movement of soil 394 water and snowmelt, as well as O<sub>2</sub> availability. Plants tends to grow better in low elevated 395 troughs with high soil water content, but aerobic respiration was suppressed by the low dissolved 396 O<sub>2</sub> concentration in saturated soils. Greater ER in high elevated ground were modeled in 397 agreement with previous studies [Zona et al., 2011]. HCP center emitted the largest emission of 398 CO<sub>2</sub> and troughs had the lowest CO<sub>2</sub> emission during growing seasons, largely caused by the 399 difference in soil O<sub>2</sub> availability for heterotrophic respiration. Obviously, ER showed a strong 400 negative response to the amount of Rubisco enzyme across the Arctic landscapes. NEE dynamics

401 was regulated by a combination of photosynthesis and respiration that produced substantial

402 uncertainties in NEE across Arctic landscape. Most landscape models do not consider the

403 microtopographic effects in simulating C fluxes. It might cause large biases; therefore, better

404 modeling microtopographic impacts on soil thermal dynamic, hydrology, and further

405 biogeochemistry is critical for model application to C cycling in the Arctic.

406

# 407 4.2. Model Performance at Different Time Steps

408 The biological processes occur at second scale, which is inconsistent with the field measurement. 409 While the ecosystem function is more important at hourly, daily, and month, and annual scale, 410 and the CLM-Microbe performance at hourly, daily, and annual time scale. The model 411 performance against observational data is more consistent with observational data at daily time 412 scale, indicating the model was not doing well in capturing some spark fluxes at hourly scale. 413 The "CH4 outbreak" in spring season has been widely recognized in recent decades [Song et al, 414 2012], that how to better simulate the outbreak events is an important topic for ecosystem 415 modeling community.

416

417 Up-scaled CH<sub>4</sub> and NEE fluxes based on the CLM-Microbe model were able to capture most 418 variations of measured EC fluxes at both daily and hourly time steps. In the EC domain, 419 dynamics of CH<sub>4</sub> and NEE at daily time step was modeled more accurately comparing with 420 simulations for hourly CH<sub>4</sub> and NEE fluxes. This is probably because the key factors or 421 processes of CH<sub>4</sub> and CO<sub>2</sub> dynamics could be slightly different across the temporal scales, but 422 they are well-defined with stable priorities in the model according to the extant knowledge 423 usually from observations at long time scales.

# 425 4.3. Model Implication

426 This study provides three implication to model developments and scientific understanding of the 427 C dynamic in the Arctic. Firstly, the CLM-Microbe performed well in capturing the variabilities 428 in CH<sub>4</sub> and CO<sub>2</sub> fluxes among primary polygonal landscapes in Arctic tundra, which emphasize 429 the importance of spatial heterogeneity in simulating CO<sub>2</sub> and CH<sub>4</sub> fluxes and should be well-430 represented in ecosystem models. Model simulated that the troughs and transitions have estimated to release CH<sub>4</sub> fluxes of  $3.6 \sim 4.0$  g C m<sup>-2</sup> y<sup>-1</sup> annually, while rims had a smaller annual 431 CH<sub>4</sub> emission of  $0.7 \sim 1.1$  g C m<sup>-2</sup> y<sup>-1</sup>. Differences in annual estimations were likely due to the 432 433 saturated and anoxic conditions in low elevational areas that promote anaerobic methanogenesis, 434 leading to a higher CH<sub>4</sub> emission. The annual CH<sub>4</sub> estimate of 2.7 g C m<sup>-2</sup> y<sup>-1</sup> for the entire study 435 area was low compared with values reported for similar ecosystems in Arctic tundra [Reeburgh 436 et al., 1998; Wille et al., 2008]. The discrepancy might be explained by the low organic matter 437 density or small proportions of PFTs in our study area; for example, the small PFTs coverage 438 shrinks the plant-mediated transport of CH<sub>4</sub> to the atmosphere that lowers CH<sub>4</sub> emission [Bhullar 439 et al., 2013]. CH<sub>4</sub> emission was recognized to have large responses to acetate production and 440 available carbon mineralization as substrate supply for methanogenesis largely relies on the 441 decomposition of soil organic matter [Kim, 2015].

442

443 Second, the potential shifts in Arctic tundra ecosystem as C sink or source is valuable

444 information for climate projection. This study showed that troughs are the only net CO<sub>2</sub> sink

445 among all landscape types and play an important role in ecosystem C storage due to its high areal

446 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 447 448 related to C mineralization and distribution among the soil C pools. It suggests that troughs 449 would rapidly shift to a net C source even with a small-scale change in C cycling in response to 450 global warming. Annual estimations indicated that HCPs had a higher strength of CO<sub>2</sub> source 451 than LCPs, which was 310% higher than LCPs. Additionally, greater ER was estimated in HCPs 452 than LCPs, and HCP center had the greatest ER of 928.0 g C m<sup>-2</sup> comparing with other landscape 453 types. Since LCPs may eventually subside into HCPs, CO<sub>2</sub> emission from Arctic soils tends to 454 increase fast not only because of effects of climate changes but also changes in landscape 455 patterns.

456

457 Last but not the least, this study advocates the mechanistic modeling of C cycling to better 458 estimate CO<sub>2</sub> and CH<sub>4</sub> fluxes across the Arctic tundra ecosystem. It is well known that 459 differences in CH<sub>4</sub> and CO<sub>2</sub> emission across the Arctic landscapes are directly led by the 460 mechanisms and dynamics of microbial activities in relation to C mineralization, decomposition, 461 respiration, methanogenesis, and methanotrophy. By inclusions of these microbial processes, the 462 CLM-Microbe model allows us to understand the mechanisms of Arctic C cycling according to 463 the production and consumption processes of CO<sub>2</sub> and CH<sub>4</sub>. Soil dissolved organic carbon 464 (DOC), CH<sub>4</sub> and CO<sub>2</sub> concentrations were modeled and compared with the measured 465 concentrations regarding the landscape types and soil depths for few data points [Yang et al., 466 2013] (Table S1). Modeled DOC concentrations were  $\sim 1.6$  times the measurements at the middle 467 layer of soils in troughs on DOY 183 and DOY 240 of 2013, which suggested that the model 468 could be useful for simulating the soil chemical concentrations. In Arctic ecosystems, large CH4 469 emission in saturated soils was modeled with great CH<sub>4</sub> production using acetic acids, which was

470 consistent with the large amount of modeled acetoclastic methanogens. CH<sub>4</sub> oxidation was 471 strengthened by high O<sub>2</sub> availability in top soils of rims and HCP center comparing with the 472 saturated troughs and transitions. Moreover, differences of CH<sub>4</sub> transport via diffusion, ebullition 473 and the plant-mediated transport were modeled with seasonal variations. Large CH<sub>4</sub> fluxes 474 emitted from soils were associated with fast plant growing during summer. Furthermore, soil 475 microbial structure and biomass can be considered to understand the CO<sub>2</sub> and CH<sub>4</sub> dynamics, by 476 model simulations for microbial biomass C and N of bacteria, fungi, acetoclastic and 477 hydrogenotrophic methanogens, aerobic and anaerobic methanotrophs.

478

#### 479 *4.4. The Way forwards*

480 The CLM-Microbe model is able to simulate the microbial processes for belowground carbon 481 cycling and surface CO<sub>2</sub> and CH<sub>4</sub> flux. Although compromising results proved the robustness of 482 the CLM-Microbe model in simulating surface CO<sub>2</sub> and CH<sub>4</sub> fluxes, a number of tasks are 483 identified as follow-up to this study. First, although the upscaling results with area-weighted 484 approach seems compromising, the dominant roles of landscape types weakened the variations in 485 C flux. An upscaling with mechanistic model should provide more accurate quantification of the 486 C flux at regional scale, as well as higher resolution C flux at both spatial and temporal scales. 487 Second, belowground C dynamics, for example, dissolved organic carbon, acetate, CO<sub>2</sub> and CH<sub>4</sub> 488 concentrations, are important variables and precursors for observed surface gas fluxes. We call 489 for a data-model integration approach to better integrate the observational data and better 490 simulate belowground processes and surface flux. Third, the hydrological dynamics is the key 491 controls to biogeochemical processes particular under the changing Arctic and the dramatic 492 impact of climate on hydrology. Improving the model's ability to better simulate hydrology is an

493 important endeavor for simulating soil biogeochemistry. Fourth, the microbial genomic 494 information is the most accurate information for microbial functions, yet it has not been well 495 utilized for model parameterization. The CLM-Microbe model is capable to simulate relative 496 abundance of methanogenesis; thus, it is worthwhile to improve the model to better simulate the 497 microbial functional groups responsible for CH<sub>4</sub> production and consumption. Fifth, although the 498 C flux data, particularly the CH<sub>4</sub> flux, has been in shortage across the Arctic tundra ecosystem, 499 recent projects and technical improvement have allowed year-round measurements. Those data 500 would be a good constrain for the CLM-Microbe model at multiple scales, therefore, a multiscale 501 "MODEX" framework to better integrate multiple sources of observational data to quantify gas 502 flux and understand their underlay mechanisms in the Arctic is needed, it should benefit the 503 scientific community.

504

#### 505 **5. Conclusions**

506 This study reported the applications of the CLM-Microbe model to seven microtopographic land 507 scape types in the Arctic tundra, Barrow, AK. The model results were promising with a 508 consistency with observational gas fluxes. Modeled results showed that low elevated landscape 509 types (troughs, transitions and LCP center) have larger CH<sub>4</sub> emission with greater seasonal 510 variations than high elevational landscape types (rims and HCP center), which was caused by the 511 higher soil saturation in the low elevated landscape types. Model sensitivity analysis showed that 512 substrate (acetate, CO<sub>2</sub>+H<sub>2</sub>) availability for methanogens was the most important factor that 513 determining CH<sub>4</sub> emission in Arctic ecosystems, and plant photosynthesis largely affected the 514 NEE and ER. The model performed better for simulating the daily EC fluxes than hourly fluxes, 515 that indicates the importance of time scale on simulating gas fluxes.

517 The CLM-Microbe model has been successfully applied to CO<sub>2</sub> and CH<sub>4</sub> fluxes in the several
518 major Arctic landscape type at the plot level. Given the large spatial heterogeneity across the
519 Arctic tundra ecosystem, it is more appropriate to conduct a mechanistic model-based upscaling
520 to estimate the ecosystem-atmosphere exchange of CH<sub>4</sub> and CO<sub>2</sub> to the EC tower and further to
521 the Pan-Arctic.

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- 529

# 530 References

- Atchley, A. L., Coon, E. T., Painter, S. L., Harp, D. R., & Wilson, C. J. (2016). Influences and
  interactions of inundation, peat, and snow on active layer thickness. Geophysical
  Research Letters, 43(10), 5116-5123.
- Bhullar, G. S., Edwards, P. J., & Olde Venterink, H. (2013). Variation in the plant-mediated
  methane transport and its importance for methane emission from intact wetland peat
  mesocosms. Journal of Plant Ecology, 6(4), 298-304.
- 537 Davidson, S. J., Sloan, V. L., Phoenix, G. K., Wagner, R., Fisher, J. P., Oechel, W. C., & Zona,
  538 D. (2016). Vegetation type dominates the spatial variability in CH4 emissions across
  539 multiple Arctic tundra landscapes. Ecosystems, 19(6), 1116-1132.
- 540 Grant, R. F. (1998), Simulation of methanogenesis in the mathematical model ecosys, Soil Biol.
  541 Biochem., 30, 883–896.
- Grant, R. F., Mekonnen, Z. A., Riley, W. J., Arora, B., & Torn, M. S. (2017). Mathematical
  modelling of arctic polygonal tundra with ecosys: 2. Microtopography determines how
  CO2 and CH4 exchange responds to changes in temperature and precipitation. Journal of
  Geophysical Research: Biogeosciences, 122(12), 3174-3187.
- Jørgensen, C. J., Johansen, K. M. L., Westergaard-Nielsen, A., & Elberling, B. (2015). Net
  regional methane sink in High Arctic soils of northeast Greenland. Nature Geoscience,
  8(1), 20.
- Kaiser, S., Göckede, M., Castro-Morales, K., Knoblauch, C., Ekici, A., Kleinen, T., ... & Wille,
  C. (2017). Process-based modelling of the methane balance in periglacial landscapes
  (JSBACH-methane). Geoscientific Model Development, 10, 333-358.
- Kettunen, A. (2003), Connecting methane fluxes to vegetation cover and water table fluctuations
  at microsite level: A modeling study, Global Biogeochem. Cycles, 17(2), 1051,
  doi:10.1029/2002GB001958.
- Kim, Y. (2015). Effect of thaw depth on fluxes of CO2 and CH4 in manipulated Arctic coastal
   tundra of Barrow, Alaska. Science of the Total Environment, 505, 385-389.
- Kumar, J., Collier, N., Bisht, G., Mills, R. T., Thornton, P. E., Iversen, C. M., & Romanovsky,
   V. (2016). Modeling the spatiotemporal variability in subsurface thermal regimes across
   a low-relief polygonal tundra landscape. The Cryosphere (Online), 10(5).
- Lau MC, Stackhouse BT, Layton AC, Chauhan A, Vishnivetskaya TA, Chourey K, Ronholm J,
   Mykytczuk NC, Bennett PC, Lamarche-Gagnon G, Burton N. An active atmospheric
   methane sink in high Arctic mineral cryosols. ISME Journal. 2015 Apr 14;1:12.
- Liljedahl, A. K., Hinzman, L. D., Harazono, Y., Zona, D., Tweedie, C. E., Hollister, R. D., ... &
  Oechel, W. C. (2011). Nonlinear controls on evapotranspiration in arctic coastal
  wetlands. Biogeosciences, 8(11), 3375-3389.
- Miller, K. E., Lai, C. T., Friedman, E. S., Angenent, L. T., & Lipson, D. A. (2015). Methane
  suppression by iron and humic acids in soils of the Arctic Coastal Plain. Soil Biology and
  Biochemistry, 83, 176-183.
- 569 Nauta, A. L., Heijmans, M. M., Blok, D., Limpens, J., Elberling, B., Gallagher, A., ... &

- 570Berendse, F. (2015). Permafrost collapse after shrub removal shifts tundra ecosystem to a571methane source. Nature Climate Change, 5(1), 67.
- Nazaries, L., Murrell, J. C., Millard, P., Baggs, L., & Singh, B. K. (2013). Methane, microbes
  and models: fundamental understanding of the soil methane cycle for future predictions.
  Environmental microbiology, 15(9), 2395-2417.
- 575 Oechel, W.C., Cowles, S., Grulke, N., Hastings, S.J., Lawrence, B., Prudhomme, T., Riechers,
  576 G., Strain, B., Tissue, D., Vourlitis, G. (1994) Transient nature of CO2 fertilization in
  577 Arctic tundra. Nature 371, 500-503.
- Olivas, P. C., Oberbauer, S. F., Tweedie, C. E., Oechel, W. C., & Kuchy, A. (2010). Responses
  of CO2 flux components of Alaskan Coastal Plain tundra to shifts in water table. Journal
  of Geophysical Research: Biogeosciences, 115(G4).
- 581 Oh, Y., Stackhouse, B., Lau, M. C., Xu, X., Trugman, A. T., Moch, J., ... & Emmerton, C. A.
  582 (2016). A scalable model for methane consumption in arctic mineral soils. Geophysical
  583 Research Letters, 43(10), 5143-5150.
- Reeburgh, W. S., King, J. Y., Regli, S. K., Kling, G. W., Auerbach, N. A., & Walker, D. A.
  (1998). A CH4 emission estimate for the Kuparuk River basin, Alaska. Journal of
  Geophysical Research: Atmospheres, 103(D22), 29005-29013.
- Riley, W. J., Subin, Z. M., Lawrence, D. M., Swenson, S. C., Torn, M. S., Meng, L., ... & Hess,
  P. (2011). Barriers to predicting changes in global terrestrial methane fluxes: analyses
  using CLM4Me, a methane biogeochemistry model integrated in CESM. Biogeosciences,
  8(7), 1925-1953.
- Segers, R. (1998), Methane production and methane consumption: A review of processes
   underlying wetland methane fluxes, Biogeochemistry, 41(1), 23–51.
- Semenchuk, P.R., Elberling, B., Amtorp, C., Winkler, J., Rumpf, S., Michelsen, A., Cooper, E.J.
  (2015) Deeper snow alters soil nutrient availability and leaf nutrient status in high Arctic
  tundra. Biogeochemistry 124, 81-94.
- Song, C., Xu, X., Sun, X., Tian, H., Sun, L., Miao, Y., Wang, X., Guo, Y. (2012) Large methane
  emission upon spring thaw from natural wetlands in the northern permafrost region.
  Environmental Research Letters 7, 10.1088/1748-9326/1087/1083/034009.
- Tan, Z., Zhuang, Q., Henze, D. K., Frankenberg, C., Dlugokencky, E., Sweeney, C., & Turner,
  A. J. (2015). Mapping pan-Arctic methane emissions at high spatial resolution using an
  adjoint atmospheric transport and inversion method and process-based wetland and lake
  biogeochemical models. Atmospheric Chemistry & Physics Discussions, 15(22).
- Taş, N., Prestat, E., Wang, S., Wu, Y., Ulrich, C., Kneafsey, T., ... & Jansson, J. K. (2018).
  Landscape topography structures the soil microbiome in arctic polygonal tundra. Nature
  communications, 9(1), 777.
- Thauer, R., D. Zinkhan, and A. Spormann (1989), Biochemistry of acetate catabolism in
  anaerobic chemotrophic bacteria, Ann. Rev. Microbiol., 43(1), 43–67.
- Thauer, R. K., A.-K. Kaster, H. Seedorf, W. Buckel, and R. Hedderich (2008), Methanogenic
  archaea: Ecologically relevant differences in energy conservation, Nat. Rev. Microbiol.,
  6(8), 579–591.

- 611 Thornton, P. E., and N. A. Rosenbloom (2005), Ecosystem model spin-up: Estimating steady
  612 state conditions in a coupled terrestrial carbon and nitrogen cycle model, Ecol. Modell.,
  613 189, 25–48.
- Thornton, P. E., J. F. Lamarque, N. A. Rosenbloom, and N. M. Mahowald (2007), Influence of
  carbon-nitrogen cycle coupling on land model response to CO2 fertilization and climate
  variability, Global Biogeochem. Cycles, 21, GB4018, doi:10.1029/2006GB002868.
- 617 Throckmorton, H. M., Heikoop, J. M., Newman, B. D., Altmann, G. L., Conrad, M. S., Muss, J.
  618 D., ... & Wilson, C. J. (2015). Pathways and transformations of dissolved methane and
  619 dissolved inorganic carbon in Arctic tundra watersheds: Evidence from analysis of stable
  620 isotopes. Global Biogeochemical Cycles, 29(11), 1893-1910.
- Tian, H., X. Xu, M. Liu, W. Ren, C. Zhang, G. Chen, and C. Lu (2010), Spatial and temporal
  patterns of CH4 and N2O fluxes in terrestrial ecosystems of North America during 1979–
  2008: Application of a global biogeochemistry model, Biogeosciences, 7, 2673–2694.
- Torn, M., Raz-Yaseef, N., & Billesbach, D. (2016). Eddy-covariance and auxiliary
  measurements, NGEE-Barrow, 2012-2013. Retrieved from http://ngee-arctic.ornl.gov/,
  accessed 5.6.2016.
- von Fischer, J. C., Rhew, R. C., Ames, G. M., Fosdick, B. K., & von Fischer, P. E. (2010).
  Vegetation height and other controls of spatial variability in methane emissions from the
  Arctic coastal tundra at Barrow, Alaska. Journal of Geophysical Research:
  Biogeosciences, 115(G4).
- Wainwright, H. M., Liljedahl, A. K., Dafflon, B., Ulrich, C., Peterson, J. E., Gusmeroli, A., &
  Hubbard, S. S. (2017). Mapping snow depth within a tundra ecosystem using multiscale
  observations and Bayesian methods. The Cryosphere (Online), 11(2).
- Walter, B. P., M. Heimann, and E. Matthews (2001), Modeling modern methane emissions from
  natural wetlands: 1. Model description and results, J. Geophys. Res., 106(D24), 34,189–
  34,206, doi:10.1029/2001JD900165.
- Wania, R., Ross, I., & Prentice, I. C. (2010). Implementation and evaluation of a new methane
  model within a dynamic global vegetation model: LPJ-WHyMe v1. 3.1. Geoscientific
  Model Development, 3(2), 565-584.
- Wille, C., Kutzbach, L., Sachs, T., Wagner, D., & PFEIFFER, E. M. (2008). Methane emission
  from Siberian arctic polygonal tundra: eddy covariance measurements and modeling.
  Global Change Biology, 14(6), 1395-1408.
- Ku, X., (2010) Modeling methane and nitrous oxide exchanges between the atmosphere and
   terrestrial ecosystems over North America in the context of multifactor global change,
   School of Forestry and Wildlife Sciences. Auburn University, Auburn, p. 199.
- Ku, X., Hahn, M. S., Kumar, J., Yuan, F., Tang, G., Thornton, P. E., ... & Wullschleger, S. D.
  (2014, December). Upscaling plot-scale methane flux to a eddy covariance tower domain in Barrow, AK: integrating in-situ data with a microbial functional group-based model. In AGU Fall Meeting Abstracts.
- Ku, X., Elias, D. A., Graham, D. E., Phelps, T. J., Carroll, S. L., Wullschleger, S. D., &
  Thornton, P. E. (2015). A microbial functional group-based module for simulating

- methane production and consumption: Application to an incubated permafrost soil.
  Journal of Geophysical Research: Biogeosciences, 120(7), 1315-1333.
- Ku, X., & Yuan, F. (2016). Meteorological forcing at Barrow AK 1981–2013. Retrieved from http://ngee-arctic.ornl.gov/. accessed 22 June 2016
- Yang, Z., Wullschleger, S. D., Liang, L., Graham, D. E., & Gu, B. (2016). Effects of warming on
  the degradation and production of low-molecular-weight labile organic carbon in an
  Arctic tundra soil. Soil Biology and Biochemistry, 95, 202-211.
- Yuan, F., Wang, G., Painter, S. L., Tang, G., Xu, X., Kumar, J., ... & Wullschleger, S. D. (2017,
  December). Effect of Freeze-Thaw Cycles on Soil Nitrogen Reactive Transport in a
  Polygonal Arctic Tundra Ecosystem at Barrow AK Using 3-D Coupled ALMPFLOTRAN. In AGU Fall Meeting Abstracts.
- Zhang, Y., Sachs, T., Li, C., & Boike, J. (2012). Upscaling methane fluxes from closed chambers
   to eddy covariance based on a permafrost biogeochemistry integrated model. Global
   Change Biology, 18(4), 1428-1440.
- Zhuang, Q., J. M. Melillo, D. W. Kicklighter, R. G. Prinn, A. D. McGuire, P. A. Steudler, B. S.
  Felzer, and S. Hu (2004), Methane fluxes between terrestrial ecosystems and the
  atmosphere at northern high latitudes during the past century: A retrospective analysis
  with a process- based biogeochemistry model, Global Biogeochem. Cycles, 18, GB3010,
  doi:10.1029/2004GB002239.
- Zona, D., Lipson, D. A., Zulueta, R. C., Oberbauer, S. F., & Oechel, W. C. (2011).
   Microtopographic controls on ecosystem functioning in the Arctic Coastal Plain. Journal
   of Geophysical Research: Biogeosciences, 116(G4).

# 674 Figure Caption

- Figure 1. The landscape classification map for Area C ( $100 \text{ m} \times 100 \text{ m}$ ). Red indicates high
- 676 surface elevation and blue indicates low surface elevation (Yuan et al., 2017).
- 677 Figure 2. Information of soil profiles and topography in study area (Yuan et al., 2017).
- 678 **Figure 3.** Modeled (a-c) CH<sub>4</sub> fluxes, (d-f) net ecosystem carbon exchange (NEE) and (g-i)
- 679 ecosystem respiration (ER) for troughs (blue lines), LCPcenter (red lines) and LCPrim (green
- 680 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) CH<sub>4</sub> fluxes, (d-f) net ecosystem carbon
- 683 exchange (NEE), and (g-i) ecosystem respiration (ER) for troughs (blue points), LCPcenter (red
- points) and LCPrim (green points), with linear lines of best fit (no interception) and 95%
- 685 confidence interval for regression line shaded grey.
- **Figure 5.** Modeled (a) CH<sub>4</sub> 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) CH<sub>4</sub> fluxes and (c, d) net ecosystem carbon exchange (NEE)
- 690 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
- 692 purple points indicate measured fluxes.
- **Figure 7.** Scatter plots of measured vs upscaled CH<sub>4</sub>(a, b) and net ecosystem carbon exchange
- 694 (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
- 696 regression line shaded grey.
- 697 **Figure 8.** Sensitivity analysis for model response of (a) CH<sub>4</sub> fluxes, (b) net ecosystem carbon
- 698 exchange (NEE) and (c) ecosystem respiration (ER) to15 parameters (KAce, ACMinQ10,
- 699 AceProdACmax, H2ProdAcemax, KH2ProdAce, KCO2ProdAce, KCO2ProdCH4,
- 700 GrowRAceMethanogens, YAceMethanogens, k\_dom, k\_bacteria, k\_fungi, flnr, grperc, br\_mr)
- 701 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
- 705 parameter change.



**Figure 1.** The landscape classification map for Area C (100 m × 100 m). Red indicates high

rog surface elevation and blue indicates low surface elevation (Yuan et al., 2017).



Figure 2. Diagram depicting the several landscape types and their soil properties along vertical

713 profiles within study area (Yuan et al., 2017)





716 **Figure 3.** Modeled (a-c) CH<sub>4</sub> fluxes, (d-f) net ecosystem carbon exchange (NEE) and (g-i)

reconsistent respiration (ER) for troughs (blue lines), LCP center (red lines) and LCP rim (green

718 lines) comparing with observed fluxes from static chambers (purple points with error bars) from

719 May to September in 2012 and 2013. Observed fluxes from Torn (2016).



Figure 4. Scatter plots of observed versus modeled (a-c) CH<sub>4</sub> fluxes, (d-f) net ecosystem carbon

- exchange (NEE), and (g-i) ecosystem respiration (ER) for troughs (blue points), LCP center (red
- points) and LCP rim (green points), with linear lines of best fit (no interception) and 95%
- 725 confidence interval for regression line shaded grey.
- 726



Figure 5. Modeled (a) CH<sub>4</sub> 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.



732

733 **Figure 6.** Upscaled (a, b) CH<sub>4</sub> fluxes and (c, d) net ecosystem carbon exchange (NEE)

- 734 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. Solid lines indicate the gas fluxes and
- 736 purple points indicate measured fluxes.





**Figure 7.** Scatter plots of measured versus upscaled CH<sub>4</sub> (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
- 742 interval for regression line shaded grey.
- 743



745 **Figure 8.** Sensitivity analysis for model response of (a) CH<sub>4</sub> fluxes, (b) net ecosystem carbon

- exchange (NEE) and (c) ecosystem respiration (ER) to15 parameters (KAce, ACMinQ10,
- 747 AceProdACmax, H2ProdAcemax, KH2ProdAce, KCO2ProdAce, KCO2ProdCH4,
- 748 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 ofparameter change.
- 754

Sites	Organic matter density (kg m <sup>-3</sup> )	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 1.** Soil organic matter and percent plant functional types (PFTs) on the natural vegetation
 land unit for all seven landscape types

Parameters Ecological meanings		
KAce	Half-saturation coefficient of available carbon mineralization	
ACminQ10	Temperature sensitivity of available carbon mineralization	
AceProdACmax	Maximum rate of acetic acid production from available carbon	
H2ProdAcemax	Maximum rate of H <sub>2</sub> production from available acetic acid	
KH2ProdAce	Half-saturation coefficient of conversion of H <sub>2</sub> and CO <sub>2</sub> to acetic acid	
KCO2ProdAce	Assuming it is half of that for H <sub>2</sub> based on stoichiometry theory	
KCO2ProdCH4	Half coefficient of CO <sub>2</sub> for methane production from H <sub>2</sub>	
GrowRAceMethanogens	Growth rate of acetoclastic methanogens	
YAceMethanogens 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 2.** Key parameters for sensitivity analysis

759 **Table 3.** Linear regression analysis for CH<sub>4</sub> fluxes, net ecosystem carbon exchange (NEE) and

reconsistent respiration (ER) modeled and observed from static chambers for troughs, LCP center

7	6	
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and LCP rim in 2012 and 2013

Variables	Sites	Estimate	Std. Error	t value	Pr(> t )	$R^2$
CH₄	Troughs	1.0008	0.1504	6.6556	0.0000*	0.7111
(2012-2013)	LCP center	1.0167	0.4683	2.1708	0.0507*	0.2820
	LCP rim	0.5023	0.2314	2.1710	0.0435*	0.2075
CH <sub>4</sub> (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
CH <sub>4</sub> (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

762 Note: "\*" indicate the significant level < 0.1.

763	Table 4. Estimation of annual budgets for CH4 fluxes, net ecosystem carbon exchange (NEE)
764	and ecosystem respiration (ER) for all seven landscape types and the EC domain based on
765	modeled daily fluxes in 2013

Sites	CH <sub>4</sub> (gC m <sup>-2</sup> yr <sup>-1</sup> )	NEE (gC $m^{-2} yr^{-1}$ )	ER (gC $m^{-2}$ yr <sup>-1</sup> )
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<sub>4</sub> 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 <sub>4</sub>	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

771 Note: "\*" indicate the significant level < 0.1.

- 772 Supplementary online materials
- 773 Table S1. The comparison between modeled and observational belowground DOC, CO<sub>2</sub>, and
- 774 CH<sub>4</sub> concentrations (gC m<sup>-3</sup>)

DOY	Sites	Sample depth (cm)	Soil layer (CLM- Microbe)	DOC		CO <sub>2</sub>		CH4	
				modeled	observed	modeled	observed	modeled	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