# **Supporting information**

This section lists the equations for representing production and consumption of CO2 and CH4, growth and death of methanogens and methanotrophy in the new CH4 module. Equations are adapted from in Xu et al. (2015) and Wang et al. (2019) with minor modifications to reflect the model application to the peatland site. All reaction processes follow the law of conservation, and the time step is semi-hourly, consistent with the ELM-SPRUCE model (Shi et al., 2015); the units for all state variables are micro-mole in one cubic meter soil/water (mmol/m3). The parameters used in the sensitivity analysis appear in red text. Note the calculations for the following equations are performed in each of the 10 model soil layers in both the hummock and hollow columns (Figure 2).

## A. Available Carbon

(S1)

*DOC* is the dissolved organic carbon, the available carbon for CH4 mechanisms; *AceProd* represent the acetate production, *CO2ProdAC*indicates the CO2 production from available carbon. The *SOM* and decomposition rate *k* used here represents the mechanism in the *Community Land Model* version 4.5 which simulates litter and soil organic matter mineralization (Koven et al., 2013; Oleson et al., 2013; Thornton & Rosenbloom, 2005). In addition to the three litter pools, four soil organic matter pools and coarse woody debris pools defined in CLM4.5, the decomposition model here is extended to include fungi, bacteria, and dissolved organic matter. For each pool *i* of the nine *Cpools* other than DOC, a portion of that pool is transferred to DOC during the decomposition process. This is determined by *ki*, the base decomposition rate of pool *i*. *Ri*, the fractional transfer from the donor carbon pool to DOC during the decomposition process, and a temperature function using a *Q10* of 1.5 (See section I). In addition to *k\_dom*, *k\_fungi* (the base turnover rate for fungi) and *k\_bacteria* (the base turnover rate for bacteria) are also varied in the sensitivity analysis.

Diffusion between vertical layers is handled by the vertical transport model introduced by Koven et al. (2013). The parameter controlling the diffusivity for dissolved organic matter (*dom\_diffus*) is varied in the sensitivity analysis.

## B. Acetate Production (Fermentation)

Below the water table, when O2 is very low, the dissolved organic carbon was fermented into acetate, carbon dioxide and H2 as the following equation:

(S2)

The acetates will be decomposed by microbe to form CH4 and CO2, and the H2 will be oxidized to CH4 if the ambient electron acceptor is scare. The following equation was used to represent the reaction under anaerobic condition.

(S3)

(S4)

(S5)

where *m\_AceProdmax* is the maximum rate and *m\_dkAce* is the half-saturation coefficient of acetate production. The *m\_dACMinQ10* is the temperature sensitivity of available carbon mineralization, *f(pH)* is the function of pH effect on acetate production, *H2ProdAC* is the H2 production and *CO2ProdAC* is the CO2 production during mineralization of available carbon.

Under aerobic condition, the available carbon was decomposed into acetate and carbon dioxide.

(S6)

(S7)

where O2 is the oxygen concentration and *AceProdQ10* is the temperature sensitivity of acetate production.

The produced H2 and CO2 will be converted to acetate or CH4 depending on the concentration of H2 (Conrad, 1989). If H2 concentration is above 340-620 nmol/L (a parameter for calibration upon simulation), the H2 and CO2 will be converted to acetate.

(S8)

(S9)

where *AceProdH2* is the acetate production from H2, *m\_dH2ProdAcemax* is the maximum potential rate of acetate production form H2, *H2*is the concentration of H2, *CO2* is the concentration of CO2, the *m\_dH2AceProdQ10* is the temperature sensitivity of homoacetogenesis, the *frace* is the function for representing homoacetogenesis dependent on H2 concentration, and the *AceH2min* represents the minimum H2 concentration above which the homoacetogenesis occurs.

If H2 concentration is below 340-620 nmol while above 16-65 nmol/L (a parameter for calibration upon simulation), the H2 and CO2 will be converted to CH4 (Conrad, 1989).

(S10)

(S11)

where *CH4ProdH2* is the CH4 production from H2 (hydrogenotrophic methanogenesis), *GrowRH2Mehtanogens* is the growth rate of hydrogenotrophic methanogens, and *YH2Mehtanogens* is the growth efficiency indicating portion of CO2 assimilated in microbes, *H2Methanogens* is the microbial biomass (active portion) of methanogens based on H2/CO2, *KH2ProdCH4* is the half-saturation coefficient of H2 used in methanogenesis, *KCO2ProdCH4* is the half-saturation coefficient of CO2 used in methanogenesis, *H2CH4ProdQ10* is the temperature sensitivity of hydrogenotrophic methanogenesis, the *frch4* is the scalar for hydrogenotrophic methanogenesis, and *CH4H2min* is the parameter below which the hydrogenotrophic methanogenesis terminates.

## C. H2 Dynamics

(S12)

(S13)

(S14)

where *H2Cons* is the consumption of H2, *H2Planttrans* is the release of H2 through the plant, *H2Dif* is the diffusion of H2, *Rootp* is the fraction of root in the soil layer in the calculation. *RootFactor* is the seasonal variation of root. is the threshold of H2 above which the H2 will be released through roots. *m\_dPlantTrans* is the efficiency for plant transport.

## D. Homoacetogenesis

(S15)

(S16)

Where *m\_dGrowRAceMethanogens* is the growth rate of hydrogenotrophic methanogens, and *YAceMethanogens* is the growth efficiency indicating portion of acetate assimilated in microbes, *AceMethanogens* is the microbial biomass of acetoclastic methanogens, *KCH4ProdAce* is the half-saturation of efficiency of acetic acid used in acetoclasitc methanogenesis, *m\_dCH4ProdQ10* is the temperature sensitivity of acetoclasitc methanogenesis.

## E. Methane

(S17)

(S18)

(S19)

(S20)

(S21)

(S22)

where *CH4Oxid* is the oxidation of CH4, *CH4Ebull* is the ebullition of CH4 release, and *CH4Dif* is the diffusion of CH4, *rCH4Prod* is growth rate of methanogens based on H2/CO2, *m\_dGrowRMethanotrophs* is the growth rate of methanotrophy, *YMethanotrophs* is the growth efficiency indicating portion of CH4 assimilated in microbes, *Methanotrophs* is the microbial biomass of methanotrophy, *KCH4OxidCH4* is the half-saturation of efficiency for CH4 in methanotrophy, K*CH4OxidO2* ishalf-saturation of efficiency for O2 in methanotrophy. The *m\_dCH4OxidQ10* is the temperature sensitivity of methanotrophy. is the threshold of CH4 above which the CH4 will be transported through plant aerenchyma. *Punveg* is the fraction of land surface which is not vegetation-covered. *m\_dCH4min* is the minimum CH4 solubility.

## F. Oxygen

(S23)

(S24)

(S25)

(S26)

where *O2PlantFlux* is the plant-mediated transport of O2, *AerO2Cons*is the oxygen oxidation during aerenchyma transport. O2*dif* is the diffusion of O2. is the threshold of O2 below which O2 will be transported from atmosphere to the deep soil.

## G. Carbon Dioxide

(S27)

(S28)

(S29)

(S30)

where *CO2Prod* is the production of CO2, *CO2Dif*is the diffusion of CO2. is the threshold of CO2 above which the CO2 will be released through root.

## H. Microbial Dynamics

(S31)

(S32)

(S33)

(S34)

(S35)

(S36)

(S37)

(S38)

(S39)

where *AceMethanogenGrowth* is the growth and *AceMethanogenDying* is the death of acetoclastic methanogens; *H2MethanogenGrowth* is the growth and *H2MethanogenDying* is the death of hydrogenotrophic methanogens; *MethanotrophGrowth* is the growth and *MethanotrophDying* is the death of methanotrophs. These equations for growth and death of various microbial functions groups were adopted from (Kettunen, 2003). The parameters are (the acetoclastic methanogen death rate), (the hydrogenotrophic methanogen death rate), (the growth efficiency of anaerobic methanotrophs), and (the methanotroph death rate).

## I. Environmental Controls

(S40)

(S41)

(S42)

(S43)

(S44)

where is the *Tsoil* is the soil temperature, *Tref* is the reference temperature, *Q10* is the temperature sensitivity, *pH* is the pH value, *pHmin* is the minimum pH value for the ecological function, *pHmax* is the maximum pH value for the ecological function, *pHopt* is the optional value for ecological function, *pHi* is the original pH value when experiments start; this *f(pH)* function is adopted from (Cao, Dent, & Heal, 1995); *f(M)* is the moisture effect on soil organic matter mineralization; *F(M)ch4* is the moisture effect on CH4 production; *f(pH)ch4* is the pH effect on CH4 production and oxidation, similar to equation used in Cao et al. (1995); *psi* is the soil water potential; *minpsi* is the minimum soil water potential for microbial activity; *maxpsi* is the maximum soil water potential; beyond the *maxpasi*, the microbial activity will not change.

**References**

Cao, M. K., Dent, J. B., & Heal, O. W. (1995). Modeling methane emissions from rice paddies. *Global Biogeochemical Cycles, 9*(2), 183-195.

Conrad, R. (1989). Control of methane production in terrestrial ecosystems. In M. O. Andrease & D. S. Schimel (Eds.), *Exchange of trace gases between terrestrial ecosystems and the atmosphere* (pp. 39-58). New York: Springer.

Kettunen, A. (2003). Connecting methane fluxes to vegetation cover and water table fluctuations at microsite level: a modeling study. *Global Biogeochemical Cycles, 17*(2), doi:10.1029/2002GB001958. doi:10.1029/2002GB001958

Koven, C. D., Riley, W., Subin, Z. M., Tang, J., Torn, M. S., Collins, W. D., . . . Swenson, S. C. (2013). The effect of vertically-resolved soil biogeochemistry and alternate soil C and N models on C dynamics of CLM4. *Biogeosciences, 10*, 7109-7131. doi:doi:10.5194/bg-10-7109-2013

Oleson, K., Lawrence, D. M., Bonan, G. B., Drewniak, B., Huang, M., Koven, C. D., . . . Thornton, P. E. (2013). *Technical description of version 4.5 of the Community Land Model (CLM)*. Retrieved from Bounder, Colorado:

Shi, X., Thornton, P. E., Ricciuto, D. M., Hanson, P. J., Mao, J., Sebestyen, S. D., . . . Bisht, G. (2015). Representing northern peatland microtopography and hydrology within the Community Land Model. *Biogeosciences, 12*(21), 6463-6477.

Thornton, P. E., & Rosenbloom, N. A. (2005). Ecosystem model spin-up: estimating steady state conditions in a coupled terrestrial carbon and nitrogen cycle model. *Ecological Modelling, 189*, 25-48.

Wang, Y., Yuan, F., Yuan, F., Gu, B., Hahn, M. S., Torn, M. S., . . . Xu, X. (2019). Mechanistic Modeling of microtopographic impact on CH4 processes in an Alaskan tundra ecosystem using the CLM-Microbe model. *Journal of Advances in Modeling Earth Systems, 11*, 4228-4304. doi:10.1029/2019MS001771

Xu, X., Elias, D. A., Graham, D. E., Phelps, T. J., Carrol, S. L., Wullschleger, S. D., & Thornton, P. E. (2015). A microbial functional group based module for simulating methane production and consumption: application to an incubation permafrost soil. *Journal of Geophysical Research-Biogeosciences, 120*(6), 1315-1333. doi:10.1002/2015JG002935