

Supplementary Material

The implication of microbial and substrate limitation for the fates of carbon in different organic soil horizon types: a mechanistically based model analysis

Supplementary Table 1

The configuration of layers in the fibric horizon based on total thickness (TZ).

Supplementary Figure 1

Convergence test for the estimators of the first and total order effects on soil organic carbon in fibric horizon with their 95% confidence interval. A sample size of 2000, highlighted in the plots, is found to be sufficient for the convergence of the estimators with relatively narrow uncertainty bound.

Supplementary Notes

Additional references from model descriptions and SI figures

Model description

1. Layer setup

The soil is divided into three horizons [Yi *et al.*, 2009; Yi *et al.*, 2010], the surface live moss layer (“live”), the slightly decomposed fibrous organic layer (“fibric”), and the moderately to very decomposed amorphous organic matter layer (“humic”). The maximum total number of layers is 7, with a maximum 1 moss layer, 3 fibric layers, and 3 humic layers. Each layer has minimum thickness of 2 cm. The layers of fibric horizon are configured according to Supplementary Table S1, and are configured in a way so that the upper layers in the soil are thinner than the deeper layers. The thicknesses and number of layers in the humic horizon (Namp) are based on the thickness of the bottom layer of fibric horizon ($d_{fib,bot}$) and the total thickness of humic horizon (d_{amp}):

$$\text{Namp} \left\{ \begin{array}{ll} 1 & d_{amp} < 3d_{fib,bot} \\ 2 & 3d_{fib,bot} \leq d_{amp} < 6d_{fib,bot} \\ 3 & d_{amp} \geq 6d_{fib,bot} \end{array} \right. \quad (1)$$

If there are 2 layers in the humic horizon, the thickness is 1/3 and 2/3 of the total thickness of humic horizon, respectively; if there are 3 layers, the thickness is 1/6, 2/6 and 3/6 of the total thickness of humic horizon, respectively. At the end of each year, the model updates the soil structure based on the calculation of total thickness of each horizon. The soil structure is updated to enable soil thermal and moisture dynamics to vary with depth. The model simulates only the organic soil up to 1m.

The layer thickness is determined based on the bulk density and C fraction of each layer as

$$Z = \sum_{j=1}^3 \left(\frac{Mass_j^{Fibric} / Cfrac^{Fibric}}{BD^{Fibric}} + \frac{Mass_j^{Humic} / Cfrac^{Humic}}{BD^{Humic}} \right) \quad (2)$$

where Z is the total thickness of soil, $Mass_j$ is the sum of all C pools (SOC + MIC + SolubleC + ENZ) in layer j , $Cfrac$ is the C fraction in fibric and humic horizon, and BD is the corresponding bulk density.

2. Decomposition

The changes in microbial biomass are simulated by the subtraction of microbial death and enzyme production and the CO₂ emitted through microbial respiration from assimilated soluble C, via which O₂ is consumed to produce energy for assimilation of dissolved organic C:

$$\frac{dMIC}{dt} = ASSIM - CO_2 - DEATH - EPROD \quad (3)$$

Assimilation is a Michaelis-Menten function scaled to the pool size of microbial biomass:

$$ASSIM = V \max_{uptake} \times MIC \times \frac{[S_x]}{kM_{[S_x]} + [S_x]} \quad (4)$$

where $V \max_{uptake}$ is the maximum velocity of the enzymatic reaction when substrate is not limiting. $kM_{[S_x]}$ is the corresponding Michaelis constant. The concentration of soluble C substrates at the reactive site of the enzyme ([S_x]) is affected by soil water content, and specifically by diffusion of substrates through soil water films. [S_x] is calculated from [S_{xsoluble}] through $[S_x] = [S_{xsoluble}] \times D_{liq} \times \theta^3$, where θ is the volumetric water content of the soil, and D_{liq} is a diffusion coefficient of the substrate in liquid phase. Diffusion of soluble substrates has been shown to be related to the thickness of the soil water films, which is approximated by the cube of the volumetric water content. It is assumed that the cell surface area available for [S_x] uptake is proportional to the number of cells, and thus the microbial biomass [Davidson *et al.*, 2012]. [S_x] is assumed to be the only substrate for microbial C uptake. Similar to Davidson *et al.* [2012], the value of D_{liq} is determined by assuming the boundary condition that all soluble substrate is available at the reaction site for saturated soil (i.e., $[S_x] = [S_{xsoluble}]$).

CO₂ is produced as the part of microbial assimilated C not allocated to biomass growth. The production process follows Michaelis-Menten kinetics similar to assimilation but is controlled by the concentration of both [S_x] and O₂:

$$CO_2 = V \max_{CO_2} \times \frac{[S_x]}{kM_{[S_x]} + [S_x]} \times \frac{[O_2]}{kM_{O_2} + [O_2]} \times MIC \quad (5)$$

subsequently, carbon use efficiency (CUE) can be obtained by

$$CUE = 1 - CO_2 / ASSIM \quad (6)$$

The concentration of O_2 at the reactive site of the enzyme ($[O_2]$) depends upon diffusion for gases within the soil medium, which is modeled with a simple function of air-filled porosity: $[O_2] = D_{\text{gas}} \times 0.209 \times a^{4/3}$. D_{gas} is a diffusion coefficient for O_2 in air, 0.209 is the volume fraction of O_2 in air, and a is the air-filled porosity of the soil. The total porosity is calculated from bulk density (BD) and particle density (PD):

$$a = 1 - \frac{BD}{PD} - \theta.$$

$V \max_{\text{uptake}}$, $V \max_{CO_2}$, and $kM_{[S_x]}$ are temperature dependent. $V \max_{\text{uptake}}$ and $V \max_{CO_2}$ follow the Arrhenius equation:

$$V \max_{\text{uptake}} = V \max_{\text{uptake}_0} \times \exp\left(-\frac{Ea_{\text{uptake}}}{R \times (T_c + 273)}\right) \quad (7)$$

$$V \max_{CO_2} = V \max_{CO_20} \times \exp\left(-\frac{Ea_{CO_2}}{R \times (T_c + 273)}\right) \quad (8)$$

where $V \max_{\text{uptake}_0}$ and $V \max_{CO_20}$ are the pre-exponential coefficient (i.e., the theoretical decomposition enzymatic reaction rate at $Ea = 0$), R is the ideal gas constant ($8.314 \text{ J K}^{-1} \text{ mol}^{-1}$), T_c is the temperature in Celsius, and Ea_{uptake} and Ea_{CO_2} are the activation energy for $[S_x]$ uptake and CO_2 respiration by microbial. High activation energy indicates high temperature sensitivity but reacts slowly. $kM_{[S_x]}$ is calculated as a linear function of temperature, as adopted in *Davidson et al.*'s [2012].

$$kM_{[S_x]} = c_{kM_{[S_x]}} + m_{kM_{[S_x]}} \times T_c \quad (9)$$

where $c_{kM_{[S_x]}}$ and $m_{kM_{[S_x]}}$ are the intercept and slope parameters, respectively. kM_{O_2} is assumed to be constant with respect to temperature for the sake of model parsimony. However, kM_{O_2} could be modeled as a function of temperature when observations are available.

Microbial death is modeled as a first-order process with rate constant r_{death} [Lawrence et al., 2009]:

$$DEATH = r_{\text{death}} \times MIC \quad (10)$$

Enzyme production is modeled as a constant fraction ($r_{EnzProd}$) of microbial biomass [Lawrence *et al.*, 2009]:

$$EPROD = r_{EnzProd} \times MIC \quad (11)$$

The enzyme pool changes with enzyme production and turnover:

$$\frac{dEnz}{dt} = EPROD - ELOSS \quad (12)$$

where the turnover (ELOSS) is modeled as a first-order process with constant rate:

$$ELOSS = r_{EnzLoss} \times Enz \quad (13)$$

The changes in SOC pool varies with external inputs, enzyme turnover, inputs from dead microbial biomass ($MICtoSOC$) and decomposition loss:

$$\frac{dSOC}{dt} = inputSOC + DEATH \times MICtoSOC + ELOSS - DECAY \quad (14)$$

where enzymatic decomposition of SOC (DECAY) here is mainly referring to the process through which microbes secrete exoenzymes to convert macromolecules into soluble products (soluble C, denoted as $[S_{xsoluble}]$) that can be absorbed and metabolized by microbes. This process follows Michaelis-Menten kinetics with enzyme and substrate (here SOC) constraint:

$$DECAY = V_{max_{SOC}} \times Enz \times \frac{SOC}{kM_{SOC} + SOC} \quad (15)$$

where $V_{max_{SOC}}$ is the maximum velocity of the enzymatic reaction when substrate is not limiting and is calculated according to Arrhenius function:

$$V_{max_{SOC}} = V_{max_{SOC_0}} \times \exp\left(-\frac{Ea_{SOC}}{R \times (temp + 273)}\right) \quad (16)$$

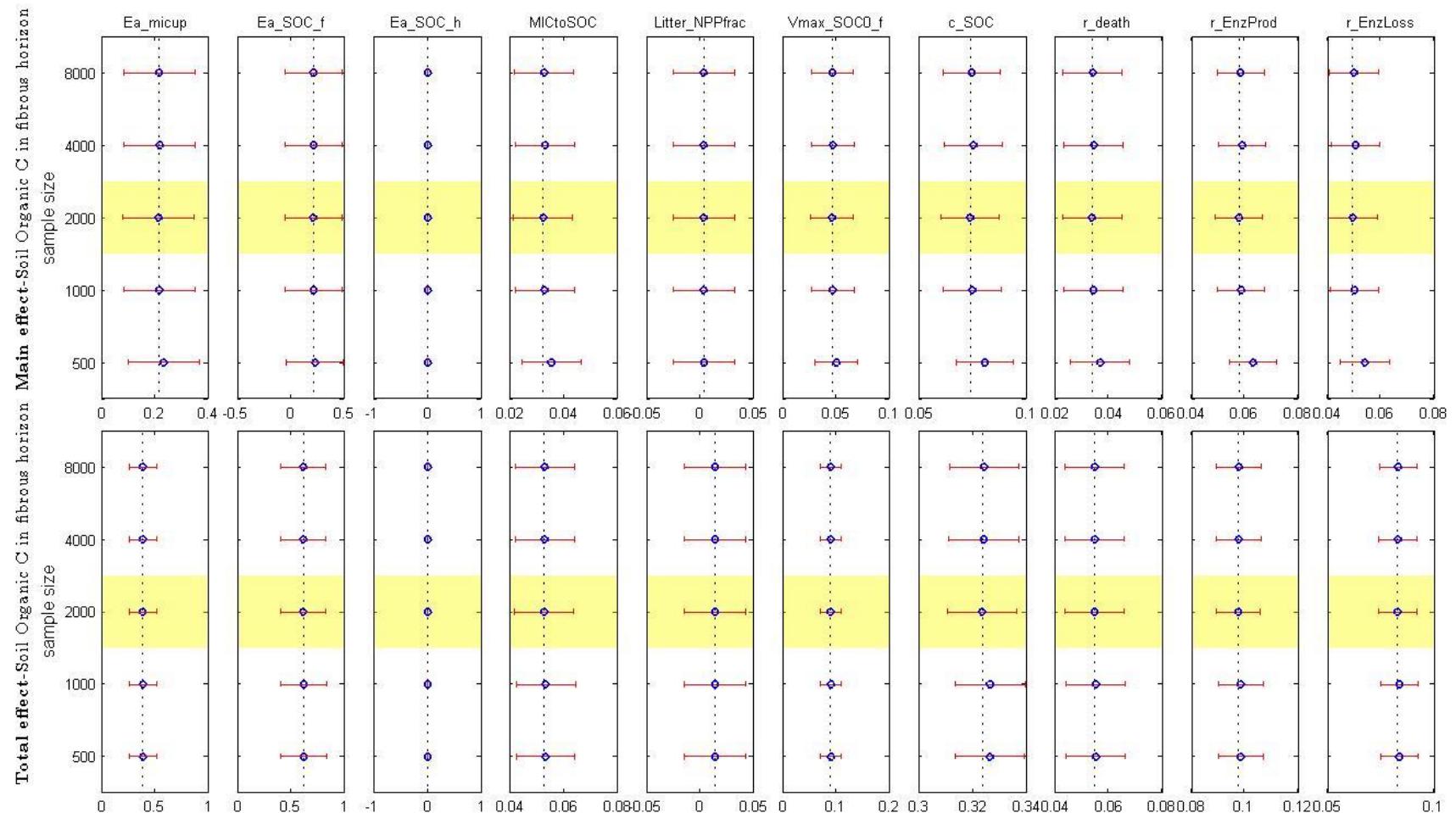
We assume Michaelis-Menten constant for SOC (kM_{SOC}) is invariable with temperature. The soluble C pool ($[S_{xsoluble}]$) changes with external inputs, the remaining fraction of dead microbial biomass, and decomposition:

$$\frac{dSolubleC}{dt} = DEATH \times (1 - MICtoSOC) + DECAY - ASSIM \quad (17)$$

This process represents the enzymatic depolymerization of complex molecules to the simpler ones available for microbial uptake.

SI Table 1.The configuration of layers in the fibric horizon based on total thickness (TZ).

Total Thickness (cm)	Layer 1	Layer 2	Layer 3 (bottom)
0~4	TZ	-	-
4~6	2	TZ-2	-
6~10	2	2	TZ-4
10~14	3	5	TZ-8
14~19	4	8	TZ-12
19~25	5	10	TZ-15
>25	6	12	TZ-18



SI Figure 1. Convergence test for the estimators of the first and total order effects on soil organic carbon in fibric horizon with their 95% confidence interval. A sample size of 2000, highlighted in the plots, is found to be sufficient for the convergence of the estimators with relatively narrow uncertainty bound.

References

Czimczik, C. I., S. E. Trumbore, M. S. Carbone, and G. C. Winston (2006), Changing sources of soil respiration with time since fire in a boreal forest, *Global Change Biology*, 12(6), 957-971.

Davidson, E. A., S. Samanta, S. S. Caramori, and K. Savage (2012), The Dual Arrhenius and Michaelis–Menten kinetics model for decomposition of soil organic matter at hourly to seasonal time scales, *Global Change Biology*.

Lawrence, C. R., J. C. Neff, and J. P. Schimel (2009), Does adding microbial mechanisms of decomposition improve soil organic matter models? A comparison of four models using data from a pulsed rewetting experiment, *Soil Biology and Biochemistry*, 41(9), 1923-1934.

Yi, S., K. Manies, J. Harden, and A. D. McGuire (2009), Characteristics of organic soil in black spruce forests: Implications for the application of land surface and ecosystem models in cold regions, *Geophysical Research Letters*, 36(5), L05501.

Yi, S., A. D. McGuire, E. Kasischke, J. Harden, K. Manies, M. Mack, and M. Turetsky (2010), A dynamic organic soil biogeochemical model for simulating the effects of wildfire on soil environmental conditions and carbon dynamics of black spruce forests, *Journal of Geophysical Research*, 115(G4), G04015.