Towards a paradigm shift in the modeling of soil organic carbon decomposition for earth system models

Yujie He
Purdue University

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TOWARDS A PARADIGM SHIFT IN THE MODELING OF SOIL ORGANIC CARBON DECOMPOSITION FOR EARTH SYSTEM MODELS

Is approved by the final examining committee:

Qianlai Zhuang
Laura Bowling
Jennifer Harden
Greg Michalski

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Qianlai Zhuang

Approved by Major Professor(s):

Approved by:

Linda Lee

Head of the Department Graduate Program

Date
I dedicate this thesis to

my parents and whom I love

for their constant support and unconditional love.

I love you all dearly.
ACKNOWLEDGEMENTS

It would not have been possible to write this doctoral thesis without the help and support of the kind people around me, to only some of whom it is possible to give particular mention here.

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ABSTRACT


Soils are the largest terrestrial carbon pools and contain approximately 2200 Pg of carbon. Thus, the dynamics of soil carbon plays an important role in the global carbon cycle and climate system. Earth System Models are used to project future interactions between terrestrial ecosystem carbon dynamics and climate. However, these models often predict a wide range of soil carbon responses and their formulations have lagged behind recent soil science advances, omitting key biogeochemical mechanisms. In contrast, recent mechanistically-based biogeochemical models that explicitly account for microbial biomass pools and enzyme kinetics that catalyze soil carbon decomposition produce notably different results and provide a closer match to recent observations. However, a systematic evaluation of the advantages and disadvantages of the microbial models and how they differ from empirical, first-order formulations in soil decomposition models for soil organic carbon is still needed. This dissertation consists of a series of model sensitivity and uncertainty analyses and identifies dominant decomposition processes in determining soil organic carbon dynamics. Poorly constrained processes or parameters
that require more experimental data integration are also identified. This dissertation also
demonstrates the critical role of microbial life-history traits (e.g. microbial dormancy) in
the modeling of microbial activity in soil organic matter decomposition models. Finally,
this study surveys and synthesizes a number of recently published microbial models and
provides suggestions for future microbial model developments.
CHAPTER 1. INTRODUCTION

1.1 Research Background

Soils are the largest carbon (C) repository in the terrestrial biosphere, releasing 60-75 Pg C to the atmosphere each year through decomposition [D S Schimel, 1995; Schlesinger and Andrews, 2000]. Previous studies suggested that decomposition rates might respond more positively to increasing temperature than photosynthetic rates [Ise et al., 2010; Mahecha et al., 2010; Smith and Dukes, 2013], potentially initiating a positive feedback between the biosphere and warming of the climate system. Thus, accurately modeling soil organic C (SOC) dynamics and microbial activity is central to understanding ecosystem responses to climate change and their feedbacks to climate. Specifically, boreal and Arctic terrestrial ecosystems in northern high latitudes are particularly sensitive to warming due to the above-global-average warming and the rich soil organic C built up in frozen soils, litter and peat [Parry et al., 2007; Tarnocai et al., 2009]. An enormous stock of C was formed in the deeper permafrost layers over tens of millennia, and both laboratory and field studies have suggested the potential rapid loss of this old C through decomposition in response to warming [Knorr et al., 2005; Schuur et al., 2009]. Annual soil respiration from temperate ecosystems accounts for about 20% of that of global total. Further, temperate ecosystems have the most field measurements comparing to boreal and tropical ecosystems [Bond-Lamberty and Thomson, 2010].
Therefore, this dissertation particularly focuses on modeling soil organic C dynamics in ecosystems of these two regions.

Current “state-of-the-art” process-based biogeochemical models are built on the basis of current consensus within the scientific community on how to represent key ecosystem processes. In modeling decomposition, the response of decomposition to temperature has traditionally been characterized with a first-order Q10 relationship that originated from empirical observations in the 19th century [van’t Hoff, 1898] and later evolved into various forms of Q10 or Arrhenius functions [Lloyd and Taylor, 1994; Sierra, 2012]. Such formulations are commonly used in contemporary biogeochemical models [Friedlingstein et al., 2006; Todd-Brown et al., 2013]. However, these models often predict a wide range of soil C responses [Todd-Brown et al., 2013] and they omit key biogeochemical mechanisms, rather based on empirical regression analyses [Conant et al., 2011; Schmidt et al., 2011]. In contrast, recent mechanistically based models that explicitly account for microbial biomass pools and enzyme kinetics that catalyze soil C decomposition produce notably different results and provide a closer match to contemporary observations [Allison et al., 2010; Wieder et al., 2013].

Although microbial models exhibit great potential for better representation of decomposition dynamics, such models usually have many parameters and some are difficult to be directly determined by measurements [Manzoni et al., 2014], thus the models can be poorly constrained. Parameter adjustments can often compensate structural uncertainties and allow model estimates to match well with observations [Beven, 2006; Bonan et al., 2011; Keenan et al., 2011; Medlyn et al., 2005]; while sensitivity analysis can help to identify the assumptions and parameters that are most influential to the
modeled system. In addition to model parameter uncertainty, model structural variation is also a major source of uncertainty. However, it is usually difficult to separate structural effects from that of parameters, a common approach to resolve this issue is to conduct simulations with a hierarchy of different model structures and compare these simulations with the same observation dataset. Subsequently, various data-assimilation techniques are developed for this purpose [Keenan et al., 2012a, Williams et al., 2009] to extract the most information for constraining models uncertainties. Ultimately, all sensitivity and uncertainty analyses and comparisons are expected to improve models’ predictability of the feedbacks between SOC dynamics and climate change.

1.2 Research Questions

This dissertation addresses the following questions:

1) What are the dominating parameters and processes in regulating soil C decomposition in fibrous and amorphous (fibric and humic in Canadian Soil Classifications, or Oi and Oa US Soil Classifications) organic soil horizons in boreal forest using mechanistically-based microbial models?

2) What are the most influential SOC decomposition processes that need critical attention in experimental work?

3) Can conceptually different SOC decomposition modeling schemes reproduce observed decomposition (heterotrophic respiration, \( R_{h} \)) from field studies?

4) How do the long-term trajectories of soil C dynamics differ among traditional Q10 and microbial decomposition models?

5) Will including microbial life history traits such as dormancy, improve model performance at both site-level and regional scales?
A series of model sensitivity and uncertainty analyses, model structure intercomparison, and model development that incorporates microbial life history traits were conducted to address the questions raised above.

1.3 Outline of Dissertation

This dissertation consists of three main chapters each corresponding to a study that addresses one or two of the research questions listed above. In Chapter 2, a multi-layer microbial explicit soil decomposition model framework was developed for boreal forest ecosystems and a thorough sensitivity analysis was conducted to identify dominating biogeochemical processes and to highlight structural limitations. In Chapter 3, three structurally different soil carbon (C) decomposition models (one Q10 and two microbial models of different complexities) were compared, each with a one- and two-horizon version. The models were calibrated and validated using four years of measurements of heterotrophic soil CO₂ efflux from trenched plots in a Dahurian larch (Larix gmelinii Rupr.) plantation. In Chapter 4, a microbial-enzyme explicit decomposition model was developed and model performance with and without representation of microbial dormancy at six temperate forest sites representing different forest types was examined. Finally, Chapter 5 summarized the major findings from previous chapters and answered the five main questions raised in Section 1.2. A survey of a dozen recently published microbial models was conducted to examine the current state of microbial modeling and mechanisms that are commonly under-represented in the majority of models. Future research directions for both modeling and experimental community were discussed.
CHAPTER 2. THE IMPLICATION OF MICROBIAL AND SUBSTRATE LIMITATION FOR THE FATES OF CARBON IN DIFFERENT ORGANIC HORIZON TYPES OF BOREAL FOREST ECOSYSTEMS: A MECHANISTICALLY BASED MODEL ANALYSIS

2.1 Abstract

The large amount of soil carbon in boreal forest ecosystems has the potential to influence the climate system if released in large quantities in response to warming. Thus, there is a need to better understand and represent the environmental sensitivity of soil carbon decomposition. Most soil carbon decomposition models rely on empirical relationships omitting key biogeochemical mechanisms and their response to climate change is highly uncertain. In this study, we developed a multi-layer microbial explicit soil decomposition model framework for boreal forest ecosystems. A thorough sensitivity analysis was conducted to identify dominating biogeochemical processes and to highlight structural limitations. Our results indicate that substrate availability (limited by soil water diffusion and substrate quality) is likely to be a major constraint on soil decomposition in the fibrous horizon (40-60% of SOC pool size variation), while energy limited microbial activity in the amorphous horizon exerts a predominant control on soil decomposition (>-70% of SOC pool size variation). Elevated temperature alleviated the energy constraint.

of microbial activity most notably in amorphous soils; whereas moisture only exhibited a marginal effect on dissolved substrate supply and microbial activity. Our study highlights the different decomposition properties and underlying mechanisms of soil dynamics between fibrous and amorphous soil horizons. Soil decomposition models should consider explicitly representing different boreal soil horizons and soil-microbial interactions to better characterize biogeochemical processes in boreal forest ecosystems. A more comprehensive representation of critical biogeochemical mechanisms of soil moisture effects may be required to improve the performance of the soil model we analyzed in this study.

2.2 Introduction

Decomposition of the large stocks of soil organic matter in northern high latitude ecosystems in response to warming is one of the largest potential feedbacks to climate change [Bond-Lamberty and Thomson, 2010; Tarnocai et al., 2009]. The already significant and expected to be more pronounced warming in the Arctic regions [ACIA, 2004] in conjunction with the large carbon (C) storage in northern permafrost soils (1104 - 1672 Pg, 50% of total global belowground organic C. Tarnocai et al., 2009; Hugelius et al., 2014) makes the understanding of how soil decomposition responds to warming climate in boreal regions an increasingly critical issue. Regional and global scale soil C models (e.g. earth system models) are often used to project future feedbacks between terrestrial ecosystem C cycle and climate. However, these models often predict a wide range of soil C response [Todd-Brown et al., 2013] and they omit key biogeochemical mechanisms based on empirical regression analyses [Conant et al., 2011; Schmidt et al., 2011]. In contrast, recent mechanistically based models that explicitly account for
microbial biomass pools and enzyme kinetics that catalyze soil C decomposition produce notably different results and provide a closer match to contemporary observations [Allison et al., 2010; Wieder et al., 2013].

Although microbial models exhibit great potential for better representation of decomposition dynamics, such models usually have many parameters and some are difficult to be directly determined by measurements [Manzoni et al., 2014], thus the model can be poorly constrained when used in real applications. In contrast to parameter adjustments which can often compensate structural uncertainties and generate satisfactory model performance that matches well with observations [Beven, 2006; Bonan et al., 2011; Keenan et al., 2011; Medlyn et al., 2005], sensitivity analysis helps to identify the assumptions and parameters that have the most important weight in the modeling system. Such information can guide critical experimental work to inform the model (especially the most influential parameters) and help better constrain the model. Sensitivity analysis thus helps to quantify the contribution of the various sources of uncertainty to the model output and also to quantify the relative importance of the assumptions, to highlight model limitations, and to provide direction for further modeling improvements as well as experimental efforts [Medlyn et al., 2005; Saltelli and Scott, 1997; Saltelli et al., 2000].

In addition, for soil decomposition models that explicitly represent microbial physiology, enzymatic activity, the direct effects of temperature and soil moisture on substrate diffusion and availability [Davidson et al., 2005; Schimel and Weintraub, 2003], and the heterogeneity of soil organic C (substrate quality and availability, and temperature sensitivity) [Davidson and Janssens, 2006; Knorr et al., 2005], we postulate that a
thorough sensitivity analysis can reflect the sensitivity of the real processes and thus help to better understand the dynamics of decomposition and its dominating factors.

In this study, we developed a mechanistically based soil decomposition modeling framework based on the multi-layer soil vertical architecture in Yi et al. [2009] to represent soil C dynamics for boreal forest ecosystems. This framework incorporates the Dual Arrhenius and Michaelis-Menten kinetics model proposed by Davidson et al. [2012] and the generic microbial-enzyme model of Allison et al. [2010] to explore the underlying mechanisms of soil respiration. This model framework is built upon the existing biochemical kinetics theory (Arrhenius and Michaelis-Menten type of functions), and explicitly represents the direct impact of temperature and moisture on biochemical reactions and the indirect effects on soil decomposition via substrate availability, enzyme activities and microbial physiology. We first calibrated the model against observed soil respiration data, we then conducted a sensitivity analysis to evaluate model limitations and gain heuristic understanding of the processes and mechanisms to further improve the model. Elevated temperature and altered moisture regimes were simulated to elucidate the impact of temperature and soil moisture on dominant decomposition processes. In particular, the following questions are addressed: 1) is this modeling framework able to reflect the sensitivity of the real processes to environmental conditions? 2) what are the dominating parameters and processes in regulating soil C decomposition in fibrous and amorphous (fibric and humic in Canadian Soil Classifications, or Oi and Oa US Soil Classifications) organic soil horizons? and 3) what are the most influential parameters or processes that need critical attention in experimental work? Specifically, the sensitivity analysis will help to evaluate 1) how well the model structure represents the real soil
decomposition processes; 2) the factors that mostly contribute to the output variability (thus the processes where accurate parameterization is critical); and 3) the important interactions among factors in the model.

2.3 Methods

2.3.1 Model Description

We simulate the soil using general organic horizon types to represent vertical soil heterogeneity in boreal ecosystems [Yi et al., 2009] (Figure 2.1). The three soil horizon types are 1) live moss at the surface (“live”); 2) slightly decomposed, fibrous organic layer made up of both dead moss and live/dead roots (“fibrous”); and 3) moderately to highly decomposed amorphous organic material (“amorphous”). Note that in the study, only heterotrophic respiration (i.e. soil organic C mineralization in fibrous and amorphous horizons) is analyzed; autotrophic respiration from live roots is not presented. Fibrous and amorphous horizons are subdivided into a maximum of three layers each based on the total thickness of a soil organic horizon, similar to the structure of soil organic horizons in Yi et al., [2010]. This architecture of layers is typical for boreal black spruce (Picea mariana (Mill.) BSP) forests, one of the major boreal forest ecosystem types in North America [Yarie, 2000]. The model simulates soil C dynamics in organic layers up to 1m in thickness. The thickness of a layer can be modified for application in other ecosystems. Temperature and moisture profiles are depth dependent variables needed for modeling soil C dynamics in each layer (see below). Each layer of fibrous and amorphous horizons consists of four C pools: soil organic C pool (SOC), soluble C pool (solubleC), microbial biomass C pool (MIC), and enzyme C pool (ENZ) (Figure 2.2).
Figure 2.1 Schematic representation of the soil decomposition model.
**Figure 2.2** Conceptual representation of soil decomposition dynamic in each layer.

Rectangles represent stocks; solid arrows denote C flows; dashed arrows represent other controls.
Litterfall, as part of C input to the soil in addition to root exudates, is prescribed as a portion of net primary production (NPP) and contributes to the fibrous and amorphous horizon with 70% and 30% respectively (follows the fine root distribution of black spruce in Canadian boreal regions [Steele et al., 1997]. Since only C is simulated, the model implicitly assumes a constant C: Nitrogen (N) ratio for each pool in the system and the effect of changes in N limitation is not simulated. C transport and conversion between pools are simulated with Arrhenius/Michaelis-Menten type equations, except for enzyme production and turnover, which is modeled as a prescribed portion of the enzyme pool.

The enzymatic decay of SOC where polymer breakdown into monomers, microbial assimilation of the dissolved organic C, and microbial respiration are simulated as:

\[ \text{DECAY} = V_{\text{max}_{\text{SOC}}} \times Enz \times \frac{SOC}{kM_{\text{SOC}} + SOC} \]  
\[ (2.1) \]

\[ \text{ASSIM} = V_{\text{max}_{\text{uptake}}} \times MIC \times \frac{[S_x]}{kM_{[S_x]} + [S_x]} \]  
\[ (2.2) \]

\[ CO_2 = V_{\text{max}_{\text{CO}_2}} \times \frac{[S_x]}{kM_{[S_x]} + [S_x]} \times \frac{[O_2]}{kM_{O_2} + [O_2]} \times MIC \]  
\[ (2.3) \]

where \( V_{\text{max}_{\text{SOC}}}, V_{\text{max}_{\text{uptake}}}, \) and \( V_{\text{max}_{\text{CO}_2}} \) are the maximum velocity of the corresponding reaction with a generic formula \( V_{\text{max}_x} = V_{\text{max}_x} \times \exp \left( \frac{Ea_x}{R \times (\text{temp}+273)} \right) \)

with \( x \) denoting corresponding process. Ea is the activation energy for the specific reaction (J mol\(^{-1}\)), R is the ideal gas constant (8.314 J mol\(^{-1}\) K\(^{-1}\)) and temp is the temperature in Celsius under which the reaction occurs. \( kM \) (unit substrate cm\(^{-3}\) soil) is the corresponding Michaelis-Menten constant. The concentration of dissolved organic
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 [Davidson et al., 2012]. [S_x] is calculated from [S_{xsoluble}] (total soluble C, i.e. SolubleC pool in the model) through

\[ [S_x] = [S_{xsoluble}] \times D_{liq} \times \theta^3, \]

where \( \theta \) is the volumetric water content of the soil and \( D_{liq} \) is the diffusion coefficient of the substrate in liquid phase [Davidson et al., 2012]. The soil model runs on an hourly time step driven by soil moisture, soil temperature and NPP.

Below is a detailed description of the model structure.

2.3.1.1 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 Table 2.1, 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 (\( N_{amp} \)) are based on the thickness of the bottom layer of fibric horizon (\( d_{fib,bot} \)) and the total thickness of humic horizon (\( d_{amp} \)):

\[
N_{amp} \begin{cases} 
1 & d_{amp} < 3d_{fib,bot} \\
2 & 3d_{fib,bot} \leq d_{amp} < 6d_{fib,bot} \\
3 & d_{amp} \geq 6d_{fib,bot}
\end{cases}
\]  

(2.4)
Table 2.1. The configuration of layers in the fibric horizon based on total thickness (TZ).

<table>
<thead>
<tr>
<th>Total Thickness (cm)</th>
<th>Layer 1</th>
<th>Layer 2</th>
<th>Layer 3 (bottom)</th>
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<tbody>
<tr>
<td>0~4</td>
<td>TZ</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>4~6</td>
<td>2</td>
<td>TZ-2</td>
<td>-</td>
</tr>
<tr>
<td>6~10</td>
<td>2</td>
<td>2</td>
<td>TZ-4</td>
</tr>
<tr>
<td>10~14</td>
<td>3</td>
<td>5</td>
<td>TZ-8</td>
</tr>
<tr>
<td>14~19</td>
<td>4</td>
<td>8</td>
<td>TZ-12</td>
</tr>
<tr>
<td>19~25</td>
<td>5</td>
<td>10</td>
<td>TZ-15</td>
</tr>
<tr>
<td>&gt;25</td>
<td>6</td>
<td>12</td>
<td>TZ-18</td>
</tr>
</tbody>
</table>
If there are 2 layers in the humic horizon, the thickness is 1/3 and 2/3 of the total thickness of the humic horizon, respectively; if there are 3 layers, the thickness is 1/6, 2/6 and 3/6 of the total thickness of the 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

\[
Z = \sum_{j=1}^{3} \left( \frac{\text{Mass}_j^{\text{Fibric}} / \text{Cfrac}_j^{\text{Fibric}}}{\text{BD}_j^{\text{Fibric}}} + \frac{\text{Mass}_j^{\text{Humic}} / \text{Cfrac}_j^{\text{Humic}}}{\text{BD}_j^{\text{Humic}}} \right)
\]

(2.4)

where \(Z\) is the total thickness of soil, \(\text{Mass}_j\) 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.

2.3.1.2 Decomposition

The changes in microbial biomass are simulated by the subtraction of microbial death and enzyme production and the CO\(_2\) emitted through microbial respiration from assimilated soluble C, via which O\(_2\) is consumed to produce energy for assimilation of dissolved organic C:

\[
\frac{d\text{MIC}}{dt} = \text{ASSIM} - \text{CO}_2 - \text{DEATH} - \text{EPROD}
\]

(2.5)

Assimilation is a Michaelis-Menten function scaled to the pool size of microbial biomass:
\[ ASSIM = V \max_{\text{uptake}} \times MIC \times \frac{[S_x]}{kM_{[S_x]} + [S_x]} \]  

(2.6)

where \( V \max_{\text{uptake}} \) 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 \([S_{\text{xsoluble}}]\) through \([S_x] = [S_{\text{xsoluble}}] \times D_{\text{liq}} \times \theta^3\), where \( \theta \) is the volumetric water content of the soil, and \( D_{\text{liq}} \) 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., 2012b]. \([S_x]\) is assumed to be the only substrate for microbial C uptake. Similar to Davidson et al. [2012], the value of \( D_{\text{liq}} \) is determined by assuming the boundary condition that all soluble substrate is available at the reaction site for saturated soil (i.e., \([S_x] = [S_{\text{xsoluble}}]\)).

\( \text{CO}_2 \) 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 \( \text{O}_2 \):

\[ CO_2 = V \max_{\text{CO}_2} \times \frac{[S_x]}{kM_{[S_x]} + [S_x]} \times \frac{[O_2]}{kM_{\text{O}_2} + [O_2]} \times MIC \]  

(2.7)

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

\[ CUE = 1 - \frac{CO_2}{ASSIM} \]  

(2.8)
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: $[O_2] = D_{gas} \times 0.209 \times a^{4/3}$. $D_{gas}$ 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):

$$a = 1 - \frac{BD}{PD} - \theta$$  \hspace{1cm} (2.9)

$V_{\text{max}_{\text{uptake}}}$, $V_{\text{max}_{\text{CO}_2}}$, and $kM_{[S_x]}$ are temperature dependent. $V_{\text{max}_{\text{uptake}}}$ and $V_{\text{max}_{\text{CO}_2}}$ follow the Arrhenius equation:

$$V_{\text{max}_{\text{uptake}}} = V_{\text{max}_{\text{uptake}0}} \times \exp \left( -\frac{E_{a_{\text{uptake}}}}{R \times (T_C + 273)} \right)$$  \hspace{1cm} (2.10)

$$V_{\text{max}_{\text{CO}_2}} = V_{\text{max}_{\text{CO}_20}} \times \exp \left( -\frac{E_{a_{\text{CO}_2}}}{R \times (T_C + 273)} \right)$$  \hspace{1cm} (2.11)

where $V_{\text{max}_{\text{uptake}0}}$ and $V_{\text{max}_{\text{CO}_20}}$ are the pre-exponential coefficient (i.e., the theoretical decomposition enzymatic reaction rate at $E_a = 0$), $R$ is the ideal gas constant (8.314 J K$^{-1}$ mol$^{-1}$), $T_C$ is the temperature in Celsius, and $E_{a_{\text{uptake}}}$ and $E_{a_{\text{CO}_2}}$ are the activation energy for $[S_x]$ uptake and CO$_2$ respiration by microorganism. High activation energy indicates high temperature sensitivity but slow reactions. $kM_{[S_x]}$ is calculated as a linear function of temperature, as adopted in Davidson et al. [2012].

$$kM_{[S_x]} = c_{kM(S_x)} + m_{kM(S_x)} \times T_C$$  \hspace{1cm} (2.12)
where $c_{kM(s_t)}$ and $m_{kM(s_t)}$ 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 $r_{\text{death}}$ [Lawrence et al., 2009]:

$$DEATH = r_{\text{death}} \times MIC$$

(2.13)

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

$$EPROD = r_{\text{EnzProd}} \times MIC$$

(2.14)

The enzyme pool changes with enzyme production and turnover:

$$\frac{dEnz}{dt} = EPROD - ELOSS$$

(2.15)

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

$$ELOSS = r_{\text{EnzLoss}} \times Enz$$

(2.16)

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

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

(2.17)

where enzymatic decomposition of SOC (DEAY) 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:

\[
DECAY = V \max_{SOC} \times Enz \times \frac{SOC}{kM_{SOC} + SOC}
\]  

(2.18)

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

\[
V_{\max_{SOC}} = V_{\max_{SOC_0}} \times \exp\left( -\frac{Ea_{SOC}}{R \times (\text{temp}+273)} \right)
\]  

(2.19)

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:

\[
\frac{d\text{SolubleC}}{dt} = DEATH \times (1 - MICToSOC) + DECAY - ASSIM 
\]  

(2.20)

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

2.3.2 Inverse parameter estimation and initial values

We parameterized the model for a black spruce dominated forest ecosystem underlain by permafrost (soil or rock that remains at or below 0°C for 2 or more years at depths of about 40 cm) in central Alaska (Donnelly Flats, lat 63°51’N, long 145°42’W) [Manies et al., 2004]. Monthly soil temperature and moisture were recorded at depths of 5, 10, and 15cm for soil temperature, and 6cm for soil moisture [Wickland et al., 2010]. The temperature and moisture profile below the above mentioned depth (up to 70cm for soil temperature, 40cm for soil moisture) were specified with data from Manies et al.
[2003]. Note here that for model sensitivity analysis purpose, we used the same monthly temperature and moisture for all the days within a month, therefore the diurnal variation of soil C dynamics are not reflected in the modeling results. Although the model does not explicitly simulate permafrost dynamics, the use of measured soil temperature and moisture content implicitly accounts for seasonal freeze/thaw and their physical controls on soil decomposition (e.g., the moisture limitation imposed by permanently frozen horizons). However, we acknowledge that the seasonal freeze-thaw processes and ground ice may have a great impact on microbial activity (see section 4.2 in Discussion), which is not represented in the model. Site-level monthly NPP used in the model is specified based on Fan et al. [2008] who used data from Mack et al. [2008], where the total annual NPP (aboveground as in stem, branch and moss, plus belowground as in root) is 250 g C m\(^{-2}\) yr\(^{-1}\). Average bulk density, C fraction, and horizon thickness at the black spruce site were determined based on Maines et al. [2004] (Table 2.2). The initial pool size for MIC, SolubleC and ENZ are prescribed according to the proportion used in Allison et al. [2010]. Other SOC and microbial activity specific parameters are determined based on other studies (Table 2.3).

We used a global optimization algorithm (Shuffled complex evolution method developed at the University of Arizona [Duan et al., 1992; Duan et al., 1994]), to constrain the poorly documented Vmax-related parameters of fibrous and amorphous horizons (Vmax_uptake0, Vmax_CO20 and Vmax SOC0). The global optimization method is used to seek the minimum of a cost function defined by the sum of squared residuals:
\[
\text{Obj} = W_{\text{resp}} \times \sum_{i=1}^{k} (\text{Resp}_{\text{obs},i} - \text{Resp}_{\text{sim},i})^2 + \\
W_{\text{mic/soc}} \times \sum_{i=1}^{k} \left( \frac{\text{MIC}_{\text{sim},i}}{\text{SOC}_{\text{sim},i}} - 0.02 \right)^2 + W_{\text{cue}} \times \sum_{i=1}^{k} (\text{CUE}_{\text{sim},i} - 0.4)^2 \quad (2.21)
\]

where the simulated soil respiration is matched with observation \((\text{Resp}_{\text{sim}}, \text{Resp}_{\text{obs}})\), the ratio between MIC pool and SOC pool is assumed to fluctuate around 2%, and simulated carbon use efficiency \((\text{CUE}, 1 - \frac{\text{CO}_2}{\text{assimilation}})\) should fluctuate around 0.4 (considering potential low quality substrates in boreal forest soils. Frey et al., 2013; Manzoni et al., 2012; Sinsabaugh et al., 2013). \(W_{\text{resp}}, W_{\text{mic/soc}}, \text{and } W_{\text{cue}}\) are the weighting function set to \(6.0 \times 10^6, 1000\) and \(100\), respectively, to reconcile the different magnitudes of metrics with approximately equal weight on MIC/SOC ratio and CUE, and a higher weight on respiration. \(k\) is the number of data pairs available to compare observation and simulation. The chamber measured monthly soil respiration data during 2003 (March-October) at the black spruce site [Wickland et al., 2010] were used for the calibration. 50% of the measured total soil respiration was assumed to be heterotrophic respiration [Schuur and Trumbore, 2006; C Wang et al., 2002]. The minimized cost function featured an adjusted \(R^2\) of 0.89 and slope of 1.19 \((p<0.05)\) for simulated and observed heterotrophic soil respiration (Figure 2.3). The optimized parameters together with other parameters (Table 2.3) were then used in the global sensitivity analysis.

2.3.3 Model experimental design

We performed a global model sensitivity analysis of recorded annual temperature and moisture conditions at the black spruce site in 2003 on decomposition parameters.
Table 2.2 Bulk density, carbon fraction, horizon thickness for different organic horizon types in soil profiles of black spruce stand in this study.

<table>
<thead>
<tr>
<th></th>
<th>Fibrous</th>
<th>Amorphous</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk density (g cm(^{-3}))</td>
<td>Mean</td>
<td>0.06</td>
<td>0.28</td>
</tr>
<tr>
<td></td>
<td>STD (n)</td>
<td>0.049 (5)</td>
<td>0.097 (4)</td>
</tr>
<tr>
<td>Carbon fraction (%)</td>
<td>Mean</td>
<td>41.12</td>
<td>21.13</td>
</tr>
<tr>
<td></td>
<td>STD (n)</td>
<td>2.24 (5)</td>
<td>6.77 (4)</td>
</tr>
<tr>
<td>Particle density (g cm(^{-3}))</td>
<td>Mean</td>
<td>1.33</td>
<td>1.33</td>
</tr>
<tr>
<td></td>
<td>STD (n)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Horizon thickness (cm)</td>
<td>Mean</td>
<td>12</td>
<td>19.25</td>
</tr>
<tr>
<td></td>
<td>STD (n)</td>
<td>3.33 (4)</td>
<td>3.4 (4)</td>
</tr>
</tbody>
</table>
Table 2.3 Parameters used in the model. Inversed estimates of specific parameters and parameter range used are listed. Bolded variables are the 10 selected parameters based on the Morris elementary effect test.

<table>
<thead>
<tr>
<th>Process</th>
<th>Parameter</th>
<th>Unit</th>
<th>Initial Value</th>
<th>Description</th>
<th>Parameter range</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Assimilation</td>
<td><strong>Ea_micup</strong></td>
<td>J mol⁻¹</td>
<td>47000</td>
<td>Soluble and diffused Sx uptake by microbial</td>
<td>-</td>
<td>Allison et al., 2010</td>
</tr>
<tr>
<td></td>
<td>Vmax_uptake0_f</td>
<td>mg Sx cm⁻³ soil (mg biomass cm⁻³ soil)⁻¹ h⁻¹</td>
<td>9.97e6</td>
<td>Maximum microbial uptake rate in fibrous horizon</td>
<td>[1.0e4, 1.0e8]</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Vmax_uptake0_h</td>
<td>mg Sx cm⁻³ soil (mg biomass cm⁻³ soil)⁻¹ h⁻¹</td>
<td>5.26e6</td>
<td>Maximum microbial uptake rate in amorphous horizon</td>
<td>[1.0e4, 1.0e8]</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>c_uptake</td>
<td>mg Sx cm⁻³ soil</td>
<td>0.1</td>
<td>Temperature regulator of MM for Sx uptake by microbes (kM_uptake)</td>
<td>-</td>
<td>Allison et al., 2010</td>
</tr>
<tr>
<td></td>
<td>m_uptake</td>
<td>mg Sx cm⁻³ soil °C⁻¹</td>
<td>0.01</td>
<td>Temperature regulator of MM for Sx uptake by microbes (kM_uptake)</td>
<td>-</td>
<td>Allison et al., 2010</td>
</tr>
<tr>
<td></td>
<td><strong>Ea_Sx_f</strong></td>
<td>J mol⁻¹</td>
<td>48092</td>
<td>Activation energy of microbes assimilating Sx to CO₂ in fibrous horizon</td>
<td>-</td>
<td>Knorr et al., 2005</td>
</tr>
<tr>
<td></td>
<td><strong>Ea_Sx_h</strong></td>
<td>J mol⁻¹</td>
<td>64334</td>
<td>Activation energy of microbes assimilating Sx to CO₂ in amorphous horizon</td>
<td>-</td>
<td>Knorr et al., 2005</td>
</tr>
<tr>
<td></td>
<td>c_Sx *</td>
<td>mg assimilated Sx cm⁻³ soil</td>
<td>0.1</td>
<td>Temperature regulator of MM for microbial assimilation of Sx (kM_Sx)</td>
<td>-</td>
<td>Allison et al., 2010</td>
</tr>
<tr>
<td></td>
<td>m_Sx *</td>
<td>mg assimilated Sx cm⁻³ soil °C⁻¹</td>
<td>0.01</td>
<td>Temperature regulator of MM for microbial assimilation of Sx (kM_Sx)</td>
<td>-</td>
<td>Allison et al., 2010</td>
</tr>
<tr>
<td>Decay</td>
<td><strong>Ea_SOC_f</strong></td>
<td>J mol⁻¹</td>
<td>41000</td>
<td>Activation energy of decomposing SOC to soluble C in fibrous horizon</td>
<td>-</td>
<td>Modified from Davidson et al., 2012</td>
</tr>
<tr>
<td></td>
<td><strong>Ea_SOC_h</strong></td>
<td>J mol⁻¹</td>
<td>58000</td>
<td>Activation energy of decomposing SOC to soluble C in amorphous horizon</td>
<td>-</td>
<td>Modified from Davidson et al., 2012</td>
</tr>
<tr>
<td></td>
<td>Vmax_SOC0_f</td>
<td>mg decomposed SOC cm⁻³ soil (mg Enz cm⁻³ soil)⁻¹ h⁻¹</td>
<td>9.17e7</td>
<td>Maximum rate of converting SOC to soluble C in fibrous horizon</td>
<td>[1.0e5, 1.0e8]</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Vmax_SOC0_h</td>
<td>mg decomposed SOC cm⁻³ soil (mg Enz cm⁻³ soil)⁻¹ h⁻¹</td>
<td>3.76e7</td>
<td>Maximum rate of converting SOC to soluble C in amorphous horizon</td>
<td>[1.0e5, 1.0e8]</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>c_SOC</td>
<td>mg SOC cm⁻³ soil</td>
<td>400</td>
<td>Temperature regulator of MM for enzymatic decay of C</td>
<td>-</td>
<td>Allison et al., 2010</td>
</tr>
<tr>
<td>Column</td>
<td>Symbol</td>
<td>Unit</td>
<td>Value</td>
<td>Description</td>
<td>Source</td>
<td></td>
</tr>
<tr>
<td>--------</td>
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<td>------</td>
<td>-------</td>
<td>-------------</td>
<td>--------</td>
<td></td>
</tr>
<tr>
<td>CO₂ production</td>
<td>m_SOC</td>
<td>mg SOC cm⁻³ soil °C⁻¹</td>
<td>5</td>
<td>Temperature regulator of MM for enzymatic decay of SOC to soluble C (kM SOC)</td>
<td>- Allison et al., 2010</td>
<td></td>
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<tr>
<td></td>
<td>kM_O₂</td>
<td>cm³₂O₂ cm⁻³ soil</td>
<td>0.121</td>
<td>Michaelis-Menten constant (MM) for O₂ (at mean value of volumetric soil moisture)</td>
<td>- Davidson et al., 2012</td>
<td></td>
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<tr>
<td>CO₂ production</td>
<td>Vmax_CO₂₀₀_f</td>
<td>mg respired Sx cm⁻³ soil h⁻¹</td>
<td>1.9e7</td>
<td>Maximum microbial respiration rate in fibrous horizon</td>
<td>[1.0e6, 1.0e8] -</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Vmax_CO₂₀₀_h</td>
<td>mg respired Sx cm⁻³ soil h⁻¹</td>
<td>6.4e7</td>
<td>Maximum microbial respiration rate in amorphous horizon</td>
<td>[1.0e6, 1.0e8] -</td>
<td></td>
</tr>
<tr>
<td></td>
<td>c_Sx *</td>
<td>mg assimilated Sx cm⁻³ soil</td>
<td>0.1</td>
<td>Temperature regulator of MM for microbial respiration of assimilated Sx (kM_Sx)</td>
<td>- Allison et al., 2010</td>
<td></td>
</tr>
<tr>
<td></td>
<td>m_Sx *</td>
<td>mg assimilated Sx cm⁻³ soil °C⁻¹</td>
<td>0.01</td>
<td>Temperature regulator of MM for microbial respiration of assimilated Sx (kM_Sx)</td>
<td>- Allison et al., 2010</td>
<td></td>
</tr>
<tr>
<td>C input</td>
<td>Litter_NPPfrac</td>
<td>%</td>
<td>30</td>
<td>Fraction of NPP allocated to litterfall</td>
<td>- Fan et al., 2008</td>
<td></td>
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<tr>
<td>MIC turnover</td>
<td>MICtoSOC</td>
<td>%</td>
<td>50</td>
<td>Partition coefficient for dead microbial biomass between the SOC and Soluble C pool</td>
<td>- Allison et al., 2010</td>
<td></td>
</tr>
<tr>
<td></td>
<td>r_death</td>
<td>% h⁻¹</td>
<td>0.02</td>
<td>Microbial death fraction</td>
<td>- Allison et al., 2010</td>
<td></td>
</tr>
<tr>
<td>ENZ turnover</td>
<td>r_EnzProd</td>
<td>% h⁻¹</td>
<td>5.0e⁻⁴</td>
<td>Enzyme production fraction</td>
<td>- Allison et al., 2010</td>
<td></td>
</tr>
<tr>
<td></td>
<td>r_EnzLoss</td>
<td>% h⁻¹</td>
<td>0.1</td>
<td>Enzyme loss fraction</td>
<td>- Allison et al., 2010</td>
<td></td>
</tr>
</tbody>
</table>

* c_Sx and m_Sx are used in both assimilation and CO₂ production calculations.
Figure 2.3 Simulated versus observed soil heterotrophic respiration from chamber measured monthly soil respiration during Mar-Oct 2003 in a black spruce dominated forest site in central Alaska. Model parameters were estimated using inverse modeling to match modeled soil heterotrophic respiration with observations.
Hereafter we refer to 2003 conditions as standard. Permafrost degradation under warmer climate can lead to complex hydrological consequences with wetter or drier soil condition depending on local microtopography, hydrology, ice content, vegetation and other factors, [Jorgenson and Osterkamp, 2005; O’Donnell et al., 2012]. To test how the sensitivity of decomposition parameters may change under warmer climate and the complex moisture conditions, we also set up three scenarios for sensitivity tests: 1) elevated temperature and standard moisture; 2) elevated temperature and raised moisture; and 3) elevated temperature and lowered moisture. We raised the monthly average temperature by 3°C as the scenario of the elevated temperature, and moisture is varied by 30% around the standard value to account for the raised and lowered moisture scenarios. Such temperature and moisture perturbations are based on observed thermokarst features in interior Alaska [O’Donnell et al., 2012].

2.3.4 Model sensitivity analysis

In the sensitivity analysis, we ran the model for 5 years with the output as time series of annual pool sizes for SOC, MIC, Soluble C, and ENZ. The pool sizes from each layer (3 layers total for each horizon) in fibrous and amorphous horizons are summed up respectively as our output of interest represents the four pools in fibrous and amorphous soils. We first implemented a screening test (section 2.3.4.1) over the total 23 parameters (Table 2.3) to identify the most important parameters at low computational cost; a quantitative, explicit evaluation (section 2.3.4.2) of the importance and interactions among the selected 10 parameters (bolded in Table 2.3) was then performed to provide detailed sensitivity analysis over those most influential parameters. The theoretical basis for the need of screening test is the Pareto principle (also known as the 80-20 rule), i.e.,
80% of the variation in model outputs can be attributed to 20% of all parameters [Saltelli et al., 2000]. The identification of the few influential parameters and the noninfluential ones can help reduce the uncertainty and computational load for more explicit and computationally expensive variance-based sensitivity analysis.

A more detailed description of the theoretical background for the sensitivity analysis methods used in this study can be found in Pappas et al. [2013]. Below we briefly outlined the steps we took in this study.

2.3.4.1 Elementary effects analysis

The Morris elementary effects (EE) method for global sensitivity analysis is categorized as a one-step-at-a-time method, meaning that in each model run, only one input parameter is given a new value while other parameters remain the same [Morris, 1991]. It is a full factorial sensitivity analysis of all calibrated parameters. An analysis of variance was used to determine the significance of each parameter on the variance of model outputs of interest. The Euclidian distance from origin (0,0) of the basic statistics (\( \varepsilon = \sqrt{\mu_{EE}^* + \sigma_{EE}^2} \), where \( \mu_{EE}^* \) is the absolute value of mean \( \mu_{EE} \) and \( \sigma_{EE} \) is standard deviation of incremental ratios from each model run) is calculated as a robust sensitivity metric [Campolongo et al., 2007]. While the EE method can provide the relative importance of a given parameter over others in one sensitivity test, its sensitivity measure cannot be compared between sensitivity tests of different outputs due to its qualitative characters (e.g., a parameter scoring 0.5 on an ENZ sensitivity test is not necessarily less influential than the same parameter scoring 5 on the SOC sensitivity test), and it cannot quantify the interactions among parameters [Saltelli et al., 2000; Saltelli et al., 2004].
altered temperature and soil moisture model experiment design were also implemented on the screening test to elucidate the impact of abiotic factors on soil C dynamics. For each sensitivity test with certain model output of interest, 100 uniformly distributed parameter samples were selected from 1000 repetitions of experiment design via space-filling improvement [Campolongo et al., 2007] and a total of 100×(23+1)=2400 model runs were conducted. To maximize the sensitivity difference among parameters, the parameters were generated with 50% variation around their original values. 10 out of 23 parameters were selected as more important parameters for the relatively computationally expensive variance-based sensitivity test.

2.3.4.2 Variance-based sensitivity analysis

We applied the Quasi-Monte Carlo estimation of Sobol’s indices [Saltelli et al., 2010; Sobol et al., 2007] on parameter samples generated from low-discrepancy Sobol sequence. The parameters were designed to vary by 20% around the original values to reduce the uncertainty introduced by overestimated parameter range. The Sobol indices consist of two indices: 1) the first-order sensitivity index (i.e., main effect index) representing the contribution to the output variance of the main effect (the effect of varying the parameter $X_i$ alone) of a specific parameter; and 2) the total-order sensitivity index which accounts for not only first- but also higher-order effects in a sense that it measures the contribution to the output variance of the parameter $X_i$, including all variance caused by the interactions between $X_i$ and any other parameter/parameters.

The model was developed in C++ with ordinary differential equation solved using the Runge-Kutta-Fehlberg 4(5) method. A portable implementation of the message
passing interface, MPICH2 (1.4.1p1 with Intel 12.0.084 compiler) was used for parallel computing of parameter sweep to reduce computational cost. The sensitivity analysis was performed in the R statistical system (http://www.r-project.org). The inverse estimation of model parameters was conducted using MATLAB optimization toolbox [Mathworks, 2012a]. Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

2.4 Results

2.4.1 Morris elementary effect test

Fibrous and amorphous horizons are controlled by different parameters, and thus by different processes. Microbial biomass (MIC) in the fibrous horizon is most sensitive to parameters associated with solubilization, or the process of degrading SOC to soluble C (Ea_SOC_f and Vmax_SOC0_f, Figure 4a), likely due to the low water holding capacity/higher porosity. MIC in the fibrous horizon is also highly sensitive to the activation energy of microbial assimilation (Ea_micup) and the external C input from litterfall (litter_NPPfrac), followed by enzyme kinetics related parameters and the turnover of dead microbes to the SOC pool (MICtoSOC) (Figure 2.4a). MIC in the amorphous horizon is generally dominated by the same set of parameters controlling fibrous C dynamics, with the exception that microbial assimilation (Ea_micup) exerts a much higher control in amorphous soil while solubilization (Ea_SOC_h) is not as influential as in fibrous soil (Figure 2.4a). SOC generally resembled the sensitivity pattern of MIC except that SOC in the fibrous horizon is more sensitive to the external organic matter input (Litter_NPPfrac) (Figure 2.4b). Soluble C in the fibrous horizon does not show a notably different response among parameters, while amorphous soil was
Figure 2.4 Screening test results (sensitivity index $\varepsilon = \sqrt{\mu_{EE}^2 + \sigma_{EE}^2}$) for microbial biomass C pool (MIC) and soil organic C pool (SOC) under standard soil temperature and moisture (STDt & STDm) scenario.
Figure 2.5 Screening test results (sensitivity index $\varepsilon = \sqrt{\mu_{EE}^2 + \sigma_{EE}^2}$) for soluble C pool (Soluble C) and enzyme pool (ENZ) under standard soil temperature and moisture (STDt & STDm) scenario.
most evidently responsive to microbial assimilation (Ea_micup) followed by the solubilization process (Ea_SOC_h) (Figure 2.5a). Enzyme pool (ENZ) in general exhibited similar sensitivity patterns with that of MIC and SOC (Figure 2.5b). These results indicate that microbial assimilation and substrate availability (solubilization process) are equally important factors for amorphous soil, while substrate availability superimposed over microbial assimilation are the most important controls of decomposition in fibrous soil.

Elevated temperature has overall greater effects on parameter sensitivity than altered moisture schemes and such effects are more pronounced in amorphous soil. Elevated temperature reduced the sensitivity of activation energy parameters in microbial assimilation (Ea_micup) in both horizons, likely due to alleviated energy limitation in the microbial activity, which only further alleviated the constrain of substrate supply (decreased sensitivity to c_SOC) in amorphous soil MIC and SOC. Temperature and moisture both have a notable effect on SolubleC and ENZ in amorphous soil. Similar to MIC and SOC in amorphous soil, elevated temperature alleviated energy limitation in microbial assimilation resulting in less sensitivity to Ea_micup. Raised soil moisture content with higher substrate diffusion likely increased the substrate supply (dissolved organic C) and thus further weakened the biochemical controls of microbial assimilation. This mechanism was also confirmed as responsible for the reduced sensitivity of SolubleC and ENZ to Ea_micup as the effects of increased temperature and moisture were offset by moisture limitation under the lowered moisture scheme (Et & Lm), rendering an increased sensitivity to activation energy related parameters.
**Figure 2.6** 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.
Through the Morris’ elementary effect analysis, we selected 10 parameters (bolded in Table 2.3) out of the original 23 parameters for Sobol’ sensitivity test to further investigate their importance.

2.4.2 Sobol’ sensitivity test

A sufficiently large sample size was determined by a convergence test of sensitivity indices where sample size of 500, 1000, 2000, 4000, and 8000 were tested, respectively. The results showed that a sample size of 2000 produced similar indices to that of 4000 and 8000 and with narrower standard deviation compared with smaller sample sizes (Figure 2.6). We therefore chose sample size of 2000 to conduct the Sobol’ sensitivity test for the 10 parameters selected via the screening test. This corresponded to $2000 \times (10+2) = 24,000$ simulations.

2.4.2.1 Decomposition in current environments

In the fibrous horizon under standard temperature and moisture scenario, about 50-90% of the variability in the pool sizes of MIC, SOC, Soluble C and ENZ can be explained by the uncertainty of $E_a_{micup}$, $E_a_{SOC_f}$, MICtoSOC and enzyme turnover related parameters respectively (Figure 2.7b). Slightly less than half of this variability (20-40%) is attributed to first-order effects (Figure 2.7a) while the rest was due to interactions with other parameters (Figure 2.7b). $c_{SOC}$ and enzyme kinetics related parameters ($r_{EnzProf}$, $r_{EnzLoss}$) also explained about 10-40% of the variability of four pools in the fibrous horizon, with the interactive effects mostly exhibited in SOC and ENZ (first order index less than half of total) (Figure 2.7). These interactions indicate a tight coupling between soil C decomposition and microbial extracellular hydrolytic enzymes. In the amorphous horizon, the majority (>80% of total effect) of the variability
Figure 2.7 Sobol’s estimates of first (a) and total order (b) parameter sensitivity indices of microbial biomass (MIC), soil organic C (SOC), soluble C (SolubleC), and enzyme (ENZ) pools with their 95% confidence intervals (vertical lines) under standard soil temperature and moisture (STDt & STDm). 8 out of 10 selected parameters are presented here because the rest 2 (Litter_NPPfrac and Vmax_SOC0_f) did not show significant sensitivity (sensitivity indices <0.1).
Figure 2.8 Coxcomb plot of Sobol’s estimates of total order parameter sensitivity indices for microbial biomass (MIC), soil organic C (SOC), soluble C (SolubleC), and enzyme (ENZ) pools under three altered environmental scenarios: elevated temperature and standard moisture (Et & STDm), elevated temperature and elevated moisture (Et & Em), elevated temperature and lowered moisture (Et & Lm) for fibrous horizon (first panel, (a)-(d)) and amorphous horizon (second panel, (e)-(h))
in each pool can be attributed to parameters related to microbial activity and enzyme turnover (Ea_micup, MICtoSOC, r_EnzProd or r_EnzLoss) (Figure 2.7b). Ea_micup, MICtoSOC and r_death exerted half of their impacts on MIC and SOC via interactions with other parameters. Soluble C in amorphous soil was almost exclusively controlled by Ea_micup with the first order index responsible for about 70% of the pool size variability (Figure 2.7a), while interactions with other parameters only added less than 5% (Figure 2.7b), suggesting the paramount importance of microbial assimilation to the simulated soluble C pool size. ENZ pool was largely controlled by parameters related to enzyme turnover (r_EnzLoss and r_EnzProd) and soil enzymatic decay (Ea_SOC_f) with the majority of contribution coming from interactive effects (first order index less than half of total).

2.4.2.2 Decomposition in altered environments

The general pattern of sensitivity in fibrous and amorphous horizons is similar to that under the standard environment except for several distinctions in response to altered temperature and moisture level. MIC and SOC in the fibrous horizon was primarily controlled by solubilization with high sensitivity to Ea_SOC_f and c_SOC, followed by microbial assimilation (Ea_micup) (Figure 2.8a,b), while the amorphous horizon was predominantly regulated by microbial dynamics related processes (Ea_micup, MICtoSOC and r_death) (Figure 2.8e,f). Increased temperature lowered the sensitivity of both horizons to activation energy terms but this effect was more notable in amorphous soil. Elevated temperature greatly reduced the sensitivity to energy threshold of microbial assimilation (Ea_micup) in the amorphous horizon by about 20% (from 0.7 in Figure 2.7b to 0.58 in Figure 2.8f Et & STDm), while only about 10% in the fibrous horizon
(from 0.38 in Figure 2.7b to 0.34 in Figure 2.8b), indicating temperature associated energy limitation could be a major cause for low microbial activity in amorphous soil. Alleviated energy limitation likely results in greater MIC biomass and subsequently raises the sensitivity to microbial turnover (r_death, Figure 2.8e,f). Altered moisture condition is expected to affect all 4 pools in the fibrous horizon, but only seems to have a slightly notable impact on Soluble C while other pools did not show a significant response (Figure 2.8c). In contrast, raised moisture likely alleviated the moisture-constrained substrate supply in the amorphous horizon and favors microbial growth, the greater MIC biomass results in higher sensitivity of parameters associated with processes of microbial activity (e.g., r_death, MICtoSOC, Figure 2.8e,f Et & STDm and Et & Em), while reduced moisture condition offset the temperature effect and yield in similar sensitivity level with that under standard environment (Figure 2.8e,f Et & Lm). The moisture response was overall less significant than the temperature effect with only marginal influence on parameter sensitivity (Figure 2.8).

2.5 Discussion

2.5.1 Different dominating process in fibrous and amorphous soils

Environmental and biological factors exert different level of controls on amorphous and fibrous soils. Amorphous soil is predominantly controlled by microbial substrate assimilation (Figure 2.4b, 2.7b), likely because the temperature induced energy limitation suppressed microbial activity. Increased moisture can alleviate the constraint to some extent, but microbial processes are still the primary controlling factors, inferred by the greater response of sensitivity to elevated temperature than to altered moisture (Figure 2.8f). In fibrous soil, which is primarily limited by substrate supply and the solubilization
process, increased moisture content does not have a significant effect on decomposition (Figure 2.8b). This may partly be explained by the higher porosity (low water holding capacity) of fibrous soil. However, moisture effects in this model were only weakly captured in both horizons, indicating that key moisture control pathways may be missing in the model. For example, studies in a temperature forest ecosystem demonstrated that low soil moisture can strongly limit in-situ enzyme activity in soils, compromising positive effects of warming [Steinweg et al., 2012]. This moisture effect on enzyme activity was not represented in our model. The high sensitivity of the fibrous horizon to Ea_SOC_f indicates the enzyme-accessible substrate quality is an important factor of simulated soil C decomposition in fibrous soil (Figure 2.7b).

Many microorganisms produce exoenzymes that catalyze the breakdown of complex polymers to usable monomers [Ratledge, 1993]. The importance of this enzyme kinetic process has been identified [Lawrence et al., 2009; Moorhead and Sinsabaugh, 2000] and proposed as a key mechanism for microbial C limitation due to low quality of soil or plant-derived substrate [Schimel and Weintraub, 2003]. The increased sensitivity of SOC enzymatic parameters under elevated temperature (Figure 2.7b, 2.8b,f) is in line with the established kinetic theory and with laboratory incubations or field measurements [Lenton and Huntingford, 2003; Liski et al., 2003; Lloyd and Taylor, 1994; Sanderman et al., 2003], where the larger portion of SOC converted to soluble form under elevated temperature causes larger variation in the SOC pool. The apparent limited response of fibrous soil to moisture variation in this study is likely to be directly attributed to the model structure where SOC decay is not directly regulated by soil moisture content. Such formulation is based on the concern that exoenzymes are usually released on or near the
reactive site of the enzyme and thus at the surface of substrate. In reality, reactions can continue even under relatively low soil moisture content because of exoenzymes [Lawrence et al., 2009]. In contrast to the amorphous horizon for which external C input does not have a direct impact, the high sensitivity of fibrous SOC to the litterfall C input (sensitivity measure of SOC to litterfall C input in Sobol test is small due to smaller parameter range than in screening test) indicates the importance of site productivity (e.g., leaf area index) to fibrous decomposition (see a modeling experiment in [Reichstein et al., 2003].

Our model sensitivity results suggest that while fibrous soil is dominated by extracellular enzymes catalyzing SOC decomposition, the microbial biomass’ ability to use the breakdown products (microbial assimilation) appears to be the major controlling process in deeper amorphous horizons. Note here that the intrinsic microbial assimilation potential is prescribed to be the same in the two horizons (same Ea_micup). As the polymer breakdown and microbial assimilation of breakdown products can be disconnected [Schimel and Weintraub, 2003], such apparent sensitivity of the metabolic status of microbial community may mask the control of SOC enzymatic decay process and substrate availability. This suggests that despite the recalcitrant SOC (as prescribed in the parameters for amorphous soils), in contrast with the fibrous horizon, substrate supply is not the predominant factor limiting decomposition. Instead, temperature and moisture limitation on microbial and enzyme activity and the subsequently reduced microbial population size and metabolic activities are important in the decomposition of the amorphous horizon. Our results provide a mechanistic explanation that agrees favorably with the molecular study of permafrost soils in Alaska, which concludes that
low microbial abundances and activities are likely to be the major limitations on decomposition rates [Waldrop et al., 2009]. In addition to the low temperature sensitivity of microbial-related parameters, as also suggested by Waldrop et al. (2009), our sensitivity analysis identifies the high sensitivity of SOC decomposition to moisture conditions via the control on substrate availability [Waldrop and Harden, 2008]. As microbial assimilation of DOC is directly regulated by the soil moisture content, reduced soil moisture could aggravate the limitation, making SOC decomposition even more sensitive to the microbial metabolism associated parameter (Ea_micup). Given the identified importance of microbial activities in amorphous soils and permafrost, changes in microbial composition and moisture condition may have a significant impact on soil C dynamics in boreal regions. As thawing permafrost alleviates diffusion constrains on substrate and hence enzyme activity, which concurrently enables growth of microbial biomass, permafrost degradation may generate greater SOC losses to the atmosphere [Schuur et al., 2009; Schuur et al., 2008]. The apparent response of microbial activity to moisture under thawing permafrost may also relieve the nutrient constraints on microbial assimilation, which although is not discussed in this study, may have implications for greater SOC loss via enhanced enzymatic decay [Mack et al., 2004; Schimel and Weintraub, 2003]. Our modeling framework demonstrates the importance of microbial activity in amorphous soils underlain by permafrost. This mechanism is especially crucial in simulating soil C dynamics in boreal ecosystems where fire is a key component of ecosystem dynamics [Balshi et al., 2009; Balshi et al., 2007; Kasischke and Turetsky, 2006], as postfire reduction in microbial population size may reduce the potential of soil
heterotrophs to decompose organic matter despite the warmer soil temperature in burned sites [Waldrop and Harden, 2008].

The apparent differences in sensitivity patterns between fibrous and amorphous soils should be explicitly represented in future modeling practices as soil organic matter is composed of different substrate pools exhibiting different sensitivities to environmental conditions [Conant et al., 2011; Hartley et al., 2007; Kirschbaum, 2004; Knorr et al., 2005]. Such differentiation of soil substrate pools is critical in understanding long term soil C dynamics, as soil components featured in long mean residence time (decades to centuries) comprise the majority of total soil C stocks [Conant et al., 2011]. It is worth noting here that our results showed microbial turnover (r_death) and the fate of those residues (MICtoSOC) are among the most influential parameters. This conclusion aligns well with results from other microbial model analysis (e.g. Wieder et al., 2014) and suggests the potentially important role of these processes on soil organic matter stabilization (e.g. partitioning into physically vs. chemically protected SOC pools).

2.5.2 Limitations and implications

Our modeling framework accounts for the microbial activity and the enzymatic dynamics between SOC decomposition and the microbial physiology. However, it does not encompass several critical microbial physiological traits which may influence ecosystem-level C balance consequences. The freeze-thaw cycles that often occur in high-latitude permafrost regions may remobilize previously frozen DOC stocks and induce a pulse in microbial respiration [Hicks Pries et al., 2013; Schimel and Clein, 1996; Schuur et al., 2009; Vonk et al., 2013], reduce microbial biomass [Christiansen et al., 2012], and may also alter N mineralization which subsequently will have consequences
on nutrient availability [Keuper et al., 2012; Schimel et al., 2007]. Microbial community composition changes that may be induced by disturbance such as warming, fire, and soil freeze-thaw process may also result in impacts on soil C dynamics [Billings and Ballantyne, 2013]. For example, changes in relative abundances of microbial functional groups may induce varying ability to compete for SOC and thus likely varying mass specific respiration rates, eventually leading to variation in soil respiration [Eliasson et al., 2005; Luo et al., 2001; Oechel et al., 2000]. Shifts in microbial community structure could also alter the temperature sensitivity of decomposition [Bradford et al., 2009; Bradford et al., 2008]. These complex feedback mechanisms are not included in the current model due to lack of sufficient theoretical understanding. Our results only weakly captured the effects of soil moisture on soil C mineralization as a driving variable, which can directly compromise the model’s ability to reproduce spatial patterns in soil C dynamics, as soil moisture has been shown to be an important control on heterotrophic respiration at both regional and local scales [Brito et al., 2013; le Roux et al., 2013; Suseela et al., 2012]. Incorporation of currently omitted processes and the improvement of mathematical representation in soil decomposition models may be needed. The fixed MIC/SOC and CUE in the objective function may have influenced the posterior parameters obtained. However, because this study focuses on sensitivity analysis in which we examined a relatively wide range for each parameter, our approach is appropriate in this context. Further studies should make use of time series of such information to help better constrain the model.

This study demonstrates how global sensitivity analysis can be used as a powerful tool to identify principal mechanisms of soil C dynamics under various soil and
environmental conditions and highlights critical aspects of model structure and uncertainty. The sensitivity results are particularly relevant for model parameterization as they identify critical parameters that may have a large impact on model outputs [Cacuci et al., 2005]. Such knowledge can potentially inform experimental practices about measurements that need to be taken and thus could be a powerful approach to guide data-model integration. It is worthy to note here that for model applications in ecosystems other than the one presented in this study, differences in parameter ranges could result in different sensitivity results [Wallach and Genard, 1998]. For example, we might expect moisture to have a less important role in SOC pool size variations in mesic systems than in arid ecosystems. Wallach and Genard [1998] recommend global sensitivity analysis for the detailed analysis of parameter space over the entire spectrum of plausible values. In this study, as most of the parameters (Table 2.3) are not well-documented at the site level or biome/plant-functional-type level, we therefore chose to evaluate a plausible range based on current knowledge. For future model applications, more detailed optimization may be desired for accurately estimating model parameters from observations.

2.6 Conclusion

In this study, we presented a mechanistically based soil C dynamic model and evaluated the sensitivity of SOC decomposition to temperature and moisture effects in fibrous and amorphous soil horizons via a global sensitivity analysis. Our results showed that substrate availability, limited by both soil water diffusion and substrate quality, is a major constraint on SOC decomposition in the fibrous horizon, while energy limitation induced microbial activity is a primary control in amorphous soils. The tight coupling
between soil organic matter mineralization and microbial extracellular hydrolytic enzymes is a critical process in both horizons. Elevated temperature alleviated the energy constraint of microbial activity most notably in amorphous soils; whereas moisture only exhibited a marginal effect on dissolved substrate supply and microbial activity. The apparent differences in sensitivity patterns between fibrous and amorphous soils in our results suggest that soils with different decomposition properties are controlled by different dominating processes. Soil decomposition models should consider explicitly representing different boreal soil horizons and soil-microbial interactions to better characterize biogeochemical processes in boreal forest ecosystems. A more comprehensive representation of critical biogeochemical mechanisms of soil moisture effects (e.g. plant root-soil interactions and freeze-thaw impact) may be required to improve the performance of the soil model we analyzed in this study.

2.7 Acknowledgement

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3.1 Abstract

Conventional Q10 soil organic matter decomposition models and more complex microbial models are available for making projections of future soil carbon dynamics. However, it is unclear (1) how well the conceptually different approaches can simulate observed decomposition, and (2) to what extent the trajectories of long-term simulations differ when using the different approaches. In this study, we compared three structurally different soil carbon (C) decomposition models (one Q10 and two microbial models of different complexity), each with a one- and two-horizon version. The models were calibrated and validated using four years of measurements of heterotrophic soil CO$_2$ efflux from trenched plots in a Dahurian larch (Larix gmelinii Rupr.) plantation. All models reproduced the observed heterotrophic component of soil CO$_2$ efflux, but the trajectories of soil carbon dynamics differed substantially in 100-year simulations with and without warming and increased litterfall input, with microbial models producing better agreement with observed changes in soil organic C in long-term warming.

experiments. Our results also suggest that both constant and varying carbon use efficiency are plausible when modeling future decomposition dynamics, and that the use of a short-term (e.g. a few years) period of measurement is insufficient to adequately constrain model parameters that represent long-term responses of microbial thermal adaption. These results highlight the need to reframe the representation of decomposition models and to constrain parameters with long-term observations and multiple data streams. We urge caution in interpreting future soil carbon responses derived from existing decomposition models because both conceptual and parameter uncertainty is substantial.

3.2 Introduction

Soils are the largest carbon (C) repository in the terrestrial biosphere, releasing 60-75 Pg C to the atmosphere each year through decomposition [D S Schimel, 1995; Schlesinger and Andrews, 2000]. Previous studies have suggested that decomposition rates may respond more positively to increasing temperature than photosynthetic rates [Ise et al., 2010; Mahecha et al., 2010; Smith and Dukes, 2013], potentially initiating a positive feedback between the biosphere and warming of the climate system. Thus, projected soil organic C (SOC) dynamics and microbial activity under future climate change are central to understanding ecosystem responses to climate change and their feedbacks to climate.

Current “state-of-the-art” process-based biogeochemical models are built on the basis of current consensus within the scientific community on how to represent key ecosystem processes. In modeling decomposition, the response of decomposition to temperature has traditionally been characterized with a first-order Q10 relationship that
originated from empirical observations in the 19th century [van’t Hoff, 1898] and later evolved into various forms of Q10 or Arrhenius functions [Lloyd and Taylor, 1994; Sierra, 2012]. Such formulations are commonly used in contemporary biogeochemical models [Friedlingstein et al., 2006; Todd-Brown et al., 2013]. However, significant uncertainty exists due to (1) conceptual uncertainty associated with fundamental physiological processes that determine responses of soil carbon dynamics [Wieder et al., 2013], and (2) parameter uncertainty within the same conceptual approach [Todd-Brown et al., 2013]. In addition, recent studies that reveal some discrepancies between model outputs and experimental data [Allison et al., 2010; Wieder et al., 2013] argue for a paradigm shift in representing soil C dynamics as traditional model structure may omit key mechanisms [Davidson et al., 2012a; Wieder et al., 2013], such as the ephemeral augmentation of soil respiration under warming [Luo et al., 2001; Melillo et al., 2002; Oechel et al., 2000] and the direct microbial control over soil C dynamics [Allison et al., 2010; Lawrence et al., 2009; Wieder et al., 2013].

In spite of recent advances in modeling soil C dynamics and model comparison efforts [Li et al., 2014; Tuomi et al., 2008], it is unclear whether conceptually different schemes can reproduce observed decomposition (heterotrophic respiration, \(R_{\text{H}}\)) from field studies. It is also not clear how the long-term trajectories of soil C dynamics differ among traditional Q10 and microbial decomposition models. To answer these two questions, we evaluated three conceptually different decomposition model structures, including one Q10 model and two microbial models with different complexities, using the observed \(R_{\text{H}}\) fluxes from trenched plots over a four-year period in deciduous forest. The two microbial models had different mechanistic complexities: a relatively simple 2-pool model with a
microbial biomass pool (MIC) and an SOC pool, and a more complex 4-pool microbial model which includes an additional extracellular enzyme pool (ENZ) and soluble C pool (SolubleC). Each structure was tested using one-horizon and two-horizon versions, where the two-horizon architecture was implemented to account for differences in decomposability between the O and the A horizons. For comparison, we used a one-horizon version of a Q10 model which had one uniform SOC pool, as well as a Q10 model that had three compartments (3-pool Q10 model): a highly labile fast turnover C pool, a resistant slow turnover C pool, and a passive C pool [Coleman and Jenkinson, 1996; Parton et al., 1993; Schädel et al., 2014]. We first calibrated all seven decomposition models using an inverse estimation technique. We then used the calibrated models to simulate soil C decomposition dynamics. We hypothesized that (1) all models would capture the variation in observed soil RH for the measurement period at model parameterization and validation stage; (2) conventional Q10 models would not reproduce realistic long-term SOC dynamics under warming scenarios.

3.3 Methods

3.3.1 Model description

The Q10 model follows the formulation described in Fan et al. [2008] and Wickland and Neff [2008]:

\[ k(\theta, T) = k^* \times [\theta_c^2 - (\theta - \theta_c)^2] \times Q_{10}^{(T-15 \degree C)/10} \]  

\[ \frac{dSOC}{dt} = -k \times SOC \]  

where \( \theta \) is the volumetric soil moisture, \( T \) is soil temperature (°C), \( \theta_c \) is the optimum volumetric moisture content corresponding to maximum decomposition rate, and \( k^* \) is
the optimum inherent decomposition rate at $\theta = \theta_c$ and $T=15$ °C. In the 3-pool Q10 model, $k^*$ varies among all three compartments. The simpler microbial model, which is based on German et al. [2012] (hereafter refer to GERM), is a two-pool model with microbial biomass pool (MIC) and a SOC pool. The more complex four-pool microbial model is a hybrid version based on Allison et al.’s [2010] microbial-enzyme model and Davidson et al.’s [2012a] DAMM model (hereafter refer to ALDA) (Figure 3.1). A detailed description of this model can be found in He et al. [2014a]. The two microbial models share a similar structure where SOC dynamics are directly regulated by either MIC or ENZ via a Michaelis-Menten enzyme kinetic function and the maximum reaction rate ($V_{\text{max}}$, h⁻¹) follows an Arrhenius temperature function:

$$DECAY = V_{\text{max}} 0_{\text{SOC}} \times \exp\left(-\frac{E_{a_{\text{SOC}}}}{R \times (T+273)}\right) \times Enz(or\text{MIC}) \times \frac{SOC}{k_{M_{\text{SOC}}} + SOC} \quad (3.3)$$

where $E_{a_{\text{SOC}}}$ is the activation energy for SOC decay (J mol⁻¹), $R$ is the ideal gas constant (8.314 J mol⁻¹ K⁻¹) and $T$ is soil temperature (°C) under which reaction occurs. $k_{M_{\text{SOC}}}$ (mg SOC cm⁻³ soil) is the corresponding Michaelis-Menten half-saturation constant.

To investigate whether representing depth-resolved processes influences the simulation of future SOC dynamics [Knorr et al., 2005; Yi et al., 2010], we constructed a two-horizon and a one-horizon version for each decomposition model. The two-horizon model explicitly simulates soil C dynamics in different soil horizons (i.e., O horizon, which contains discernable particulate organic matter, and A horizon, which occurs just below the O horizon). The thickness of each horizon is reassigned to different soil layers each year based on the total simulated thickness of that horizon [He et al., 2014a], thus
Figure 3.1. Schematic diagram of the three models
allowing the vertical temperature and moisture profile to correspond with changing thickness of the soil column. By distinguishing soil horizons we were also able to partition SOC into components with different intrinsic turnover rates, i.e. the more labile (O) vs. the more recalcitrant (A) SOC. The one-horizon model combines the SOC in the O and A horizon into a single horizon, and thus a single SOC pool. The 3-pool Q10 model is also one-horizon but partitions total SOC stock into three compartments with different intrinsic decomposability.

### 3.3.2 Inverse estimation of model parameters

#### 3.3.2.1 Site description and observational constraints

Soil CO₂ efflux and physical environmental data were collected at a site at the Maoershan Ecosystem Research Station in China (127°30-34’E, 45°20-25’N) dominated by Dahurian larch (*Larix gmelinii* Rupr.), a typical forest ecosystem in that region. A detailed description of site characteristics can be found in *Wang et al.* [2006]. This site has three replicate fixed plots (20m × 30m) with four R₇H sampling subplots (50cm × 50cm) which were trenched to be free of live vegetation. In each R₇H subplot one polyvinyl chloride (PVC) collar (10.2 cm inside diameter × 6 cm height) was installed [C *Wang and Yang*, 2007]. To minimize artifacts associated with trenching disturbance [Bond-Lamberty et al., 2011; Jassal and Black, 2006; Lavigne et al., 2004], we only used measured R₇H data that were collected two or more months after trenching. Soil surface CO₂ fluxes from trenched plots were measured with a Li-Cor 6400 portable CO₂ infrared gas analyzer connected with a Li-6400-09 chamber (Li-Cor Inc., Lincoln, NE, USA) biweekly from 2004 to 2007. Biweekly data were averaged to monthly resolution for consistency. Soil temperature and gravimetric water content were measured at 2cm and
10cm depths near each collar concurrently with $R_{FI}$ measurements. Soil temperature was measured with a digital long-stem thermometer. Soil water content was determined by taking soil samples at two depths and dried at 70°C to a constant mass. To account for the potential that estimated microbial respiration included decomposition of pre-existing roots [Drake et al., 2012; Graham et al., 2012], we calculated the CO$_2$ efflux caused by the decomposition of labile components from dead root detritus based on root biomass [C Wang et al., 2006], the generalized models of fine root decay rate with respect to latitude [Silver and Miya, 2001], and the published decay rate for coarse roots [Landsberg and Gower, 1997], as was done in Wang and Yang [2007]. Calculated root decay was then subtracted from measured soil CO$_2$ efflux. Note that the soil at this site contains only a minimal amount of clay. Measured thickness, bulk density, SOC content, and microbial biomass of each soil horizon were collected as initial states and fixed parameters for the models (Table 3.1) [Liu and Wang, 2010; Yang and Wang, 2005]. The light and heavy fraction of the organic matter of the O and A horizon was determined by density fractionation [Zhao, 2013]. Light fraction is regarded as highly labile whereas heavier amorphous material (heavy fraction) is regarded as more recalcitrant [Boone, 1994; Tan et al., 2007; Trumbore, 1993]. The measured light and heavy fraction of the soil was used as prior for estimating the parameters of the 3-pool Q10 model (Table 3.1).

3.3.2.2 Assimilation scheme and model validation

Under Bayesian framework, the posterior probability density function (PDF) $p_{\text{post}}$ of a sample from the joint parameter distribution $\theta$ is a function of the prior probability of joint parameter $p_{\text{prior}}$ and observation $x$:
Table 3.1 Soil physical metrics and MIC/SOC ratio of different horizon (O and A horizon) types of the needleleaf deciduous forest stand in this study.

<table>
<thead>
<tr>
<th>Metrics</th>
<th>O</th>
<th>A</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk density (g cm$^{-3}$)</td>
<td>Mean 0.87</td>
<td>1.1</td>
<td>Yang and Wang, 2005</td>
</tr>
<tr>
<td></td>
<td>STD (n) 0.45 (9)</td>
<td>0.05 (9)</td>
<td></td>
</tr>
<tr>
<td>Organic carbon fraction (%)</td>
<td>Mean 5.1</td>
<td>4.1</td>
<td>Yang and Wang, 2005</td>
</tr>
<tr>
<td></td>
<td>STD (n) 1.2 (9)</td>
<td>0.93 (9)</td>
<td></td>
</tr>
<tr>
<td>Porosity (%)</td>
<td>Mean 64.8</td>
<td>59.2</td>
<td>Fan et al., 2004</td>
</tr>
<tr>
<td></td>
<td>STD (n) -</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Particle density (g cm$^{-3}$)</td>
<td>Mean 2.47</td>
<td>2.75</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>STD (n) -</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Horizon thickness (cm)</td>
<td>Mean 4.11</td>
<td>14.22</td>
<td>Yang and Wang, 2005</td>
</tr>
<tr>
<td></td>
<td>STD (n) 1.6 (9)</td>
<td>8.47 (9)</td>
<td></td>
</tr>
<tr>
<td>MIC/SOC (%)</td>
<td>Summer Mean 0.054</td>
<td>0.045</td>
<td>Liu and Wang, 2010</td>
</tr>
<tr>
<td></td>
<td>STD (n) 0.002 (3)</td>
<td>0.001 (3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Winter Mean 0.09</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>STD (n) 0.003 (3)</td>
<td>0.002 (3)</td>
<td></td>
</tr>
<tr>
<td>Fraction of light-fraction SOM</td>
<td>Mean 0.14</td>
<td>0.04</td>
<td>Zhao, 2013</td>
</tr>
<tr>
<td></td>
<td>STD (n) 0.09 (10)</td>
<td>0.01 (10)</td>
<td></td>
</tr>
<tr>
<td>Fraction of heavy-fraction SOM</td>
<td>Mean 0.8</td>
<td>0.87</td>
<td>Zhao, 2013</td>
</tr>
<tr>
<td></td>
<td>STD (n) 0.09 (10)</td>
<td>0.05 (10)</td>
<td></td>
</tr>
</tbody>
</table>
\[ P_{\text{post}}(\theta | x) = \frac{L(x | \theta) P_{\text{prior}}(\theta)}{\int L(x | \theta) P_{\text{prior}}(\theta) d\theta} \]

The denominator on the right hand side is the marginal distribution of \( x \); therefore given a realization of observation, the denominator is a constant and then can be ignored in the optimization. We assume the prior distribution is uniform, and all observations are independently and identically distributed (IID) and follow a normal distribution, the likelihood \( L(\theta | x) \) can be formed as:

\[
L(x | \theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{1}{2} \frac{(f(\theta, t_i) - x_i)^2}{\sigma_i^2}\right]
\]

where \( n \) is the number of observations \( x_1, x_2, ..., x_n \) at time \( t_1, t_2, ..., t_n \). \( \sigma_i \) is the standard deviation of each observation due to observation noise and measurement error, thus \( \sigma_i \) can differ among individual observations. However, because we lack the information necessary to determine how \( \sigma_i \) varies with each measurement, we made a simplification to assume constant \( \sigma_i \) for all observations. Applying a ‘log-transformation’ to the likelihood and ignoring the constant terms, we obtained the following objective functions to calibrate the seven models (3 structures × 2 versions + 1 3-pool Q10) using measured trenched plot soil efflux:

ALDA:

\[
\text{Obj} = W_{exp} \times \sum_{i=1}^{l} (\text{Resp}_{obs,i} - \text{Resp}_{sim,i})^2 + W_{mic/soc} \times \sum_{i=1}^{l} \left( \frac{MIC_{sim,i,1}}{SOC_{sim,i,1}} - 0.001 \right)^2 + \\
W_{mic/soc} \times \sum_{i=1}^{l} \left( \frac{MIC_{sim,i,2}}{SOC_{sim,i,2}} - 0.0005 \right)^2 + W_{cue} \times \sum_{i=1}^{l} (\text{CUE}_{sim,i} - 0.5)^2
\]

GERM:
\[
\text{Obj} = W_{\text{resp}} \times \sum_{i=1}^{k} (\text{Re} \, \text{sp}_{\text{obs},i} - \text{Re} \, \text{sp}_{\text{sim},i})^2 + W_{\text{mic}/\text{soc}} \times \sum_{i=1}^{l} \left( \frac{\text{MIC}_{\text{sim},i}}{\text{SOC}_{\text{sim},i}} - 0.001 \right)^2 \\
+ W_{\text{mic}/\text{soc}} \times \sum_{i=1}^{l} \left( \frac{\text{MIC}_{\text{sim},i}}{\text{SOC}_{\text{sim},i}} - 0.0005 \right)^2
\]  

(3.7)

Q10: \[
\text{Obj} = W_{\text{resp}} \times \sum_{i=1}^{k} (\text{Re} \, \text{sp}_{\text{obs},i} - \text{Re} \, \text{sp}_{\text{sim},i})^2
\]  

(3.8)

where the differences between the simulated decomposition (\(\text{Re} \, \text{sp}_{\text{sim}}\)), the simulated ratio between microbial biomass and SOC (\(\frac{\text{MIC}_{\text{sim}}}{\text{SOC}_{\text{sim}}}\)) and the simulated carbon use efficiency (\(\text{CUE}_{\text{sim}}\)) and observations were minimized. The measured annual average \(\frac{\text{MIC}}{\text{SOC}}\) of O (0.001) and A (0.0005) horizons are adopted from [Liu and Wang, 2010] (for the one-horizon model, the average \(\frac{\text{MIC}}{\text{SOC}}\) was used). Simulated CUE was assumed to fluctuate around 0.5 as commonly reported in other studies [Frey et al., 2013; Manzoni et al., 2012; Sinsabaugh et al., 2013]. \(W_{\text{resp}}, W_{\text{mic}/\text{soc}}, \text{and } W_{\text{cue}}\) are the weighting function set to \(6.0 \times 10^6, 1000\) and \(100\), respectively, to reconcile the different magnitudes of metrics. \(k\) is the number of data pairs available to compare observation and simulation. See the supporting information for more details of the prior and optimized parameter values.

We applied a global optimization method known as the SCE-UA (shuffled complex evolution) [Duan et al., 1992; Duan et al., 1994], which is an effective and efficient method specifically designed to obtain global convergence in the presence of multiple regions of attraction under high-parameter dimensionality. We performed 100 independent optimization runs, each using different random number seed to determine the successive evolution steps. The resulting stationary distribution from the 100 runs...
converges to the joint parameter posterior PDF. The two-horizon ALDA model has the highest number of parameters of 16, and the simplest one-horizon Q10 model has only 3 parameters. It took on average ~200,000 and ~15,000 model evaluations to converge on the optimum parameter sets for the two models, respectively.

Because of limited data availability for calibration, we calibrated each model with the first three years of field-based decomposition estimates and validated each model with field-based decomposition estimates from the fourth year. The goodness-of-fit statistics between field-based and model simulation estimates of decomposition were calculated using all four years of estimates. Because the trenched plot does not have litter inputs, the modeling system will equilibrate when decomposition reaches zero (microbial biomass equals zero), therefore we did not start the simulation from equilibrium but rather did a one-year spin up to stabilize the pool sizes. The initial prior ranges for model parameters were obtained from literature (e.g., Allison et al. [2010], Knorr et al. [2005], and German et al. [2012]), and were later expanded or shifted during the optimization process to ensure that the posterior distribution was not truncated by the prior range (Tables 3.2-3.4).

3.3.3 Future extrapolation

To examine how structural differences can affect projection, we conducted two sets of simulations: (1) control simulations with no litterfall input or warming (i.e., the natural projection of the initial SOC of a trenched plot that is expected to decrease over time); and (2) simulations with progressively increasing litter inputs and temperature. Monthly litterfall from an adjacent control plot was collected during 2005 using mesh-gridded cloth with diameter 1m (unpublished data, Figure 3.2a). Our total annual litterfall
Figure 3.2 (a) The litterfall carbon data collected at the control site in 2005. (b) The imposed 3% increase per decade in litterfall over the warming scenario for 100 years.
Table 3.2 Parameters priors and 95% CI of posteriors of ALDA model from inverse estimation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Description</th>
<th>Prior</th>
<th>Posterior 95% CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ea_micup</td>
<td>J mol⁻¹</td>
<td>Soluble and diffused Sx uptake by microbial</td>
<td>[3.5e4, 7.5e4]</td>
<td>[5.31e4, 5.54e4]</td>
</tr>
<tr>
<td>Ea_Sx_O</td>
<td>J mol⁻¹</td>
<td>Activation energy of microbes assimilating Sx to CO₂ in O horizon</td>
<td>[3.5e4, 7.5e4]</td>
<td>[4.34e4, 4.38e4]</td>
</tr>
<tr>
<td>Ea_Sx_A0</td>
<td>J mol⁻¹</td>
<td>Activation energy of microbes assimilating Sx to CO₂ in A horizon</td>
<td>[3.5e4, 7.5e4]</td>
<td>[5.81e4, 5.94e4]</td>
</tr>
<tr>
<td>Ea_SOC_O</td>
<td>J mol⁻¹</td>
<td>Activation energy of decomposing SOC to soluble C in O horizon</td>
<td>[3.5e4, 7.5e4]</td>
<td>[2.95e4, 5.12e4]</td>
</tr>
<tr>
<td>Ea_SOC_A0</td>
<td>J mol⁻¹</td>
<td>Activation energy of decomposing SOC to soluble C in A horizon</td>
<td>[3.5e4, 7.5e4]</td>
<td>[5.43e4, 5.49e4]</td>
</tr>
<tr>
<td>Vmax_uptake0_O</td>
<td>mg Sx cm⁻³ soil (mg biomass cm⁻³ soil⁻¹ h⁻¹)</td>
<td>Maximum microbial uptake rate in O horizon</td>
<td>[9.0e6, 7.0e7]</td>
<td>[1.04e7, 3.16e7]</td>
</tr>
<tr>
<td>Vmax_uptake0_A0</td>
<td>mg Sx cm⁻³ soil (mg biomass cm⁻³ soil⁻¹ h⁻¹)</td>
<td>Maximum microbial uptake rate in A horizon</td>
<td>[9.0e6, 7.0e7]</td>
<td>[2.96e7, 6.38e7]</td>
</tr>
<tr>
<td>Vmax_CO20_O</td>
<td>mg respired Sx cm⁻³ soil h⁻¹</td>
<td>Maximum microbial respiration rate in O horizon</td>
<td>[7.0e7, 1.5e8]</td>
<td>[8.38e7, 1.25e8]</td>
</tr>
<tr>
<td>Vmax_CO20_A0</td>
<td>mg respired Sx cm⁻³ soil h⁻¹</td>
<td>Maximum microbial respiration rate in A horizon</td>
<td>[7.0e8, 1.5e9]</td>
<td>[5.93e8, 1.01e9]</td>
</tr>
<tr>
<td>Vmax_SOC0_O</td>
<td>mg decomposed SOC cm⁻³ soil (mg Enz cm⁻³ soil⁻¹ h⁻¹)</td>
<td>Maximum rate of converting SOC to soluble C in O horizon</td>
<td>[4.0e6, 1.5e8]</td>
<td>[4.64e6, 1.02e7]</td>
</tr>
<tr>
<td>Vmax_SOC0_A0</td>
<td>mg decomposed SOC cm⁻³ soil (mg Enz cm⁻³ soil⁻¹ h⁻¹)</td>
<td>Maximum rate of converting SOC to soluble C in A horizon</td>
<td>[4.0e6, 1.5e8]</td>
<td>[8.89e7, 1.26e8]</td>
</tr>
<tr>
<td>r_death</td>
<td>% h⁻¹</td>
<td>Microbial death fraction</td>
<td>[1.0e-4, 1.0e-3]</td>
<td>[3.36e-4, 7.87e-4]</td>
</tr>
<tr>
<td>r_EnzProd</td>
<td>% h⁻¹</td>
<td>Enzyme production fraction</td>
<td>[4.0e-6, 1.2e-5]</td>
<td>[6.93e-6, 1.15e-5]</td>
</tr>
<tr>
<td>r_EnzLoss</td>
<td>% h⁻¹</td>
<td>Enzyme loss fraction</td>
<td>[5.0e-4, 2.0e-3]</td>
<td>[6.59e-4, 0.0013]</td>
</tr>
</tbody>
</table>
Table 3.3 Parameters priors and 95% CI of posteriors of GERM model from inverse estimation.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Description</th>
<th>Prior</th>
<th>Posterior 95% CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ea_SOC_O</td>
<td>J mol(^{-1})</td>
<td>Activation energy of SOC decomposition in O horizon</td>
<td>[3.5e4, 7.5e4]</td>
<td>[4.81e4, 5.02e4]</td>
</tr>
<tr>
<td>Ea_SOC_A0</td>
<td>J mol(^{-1})</td>
<td>Activation energy of SOC decomposition in A horizon</td>
<td>[3.5e4, 7.5e4]</td>
<td>[5.85e4, 7.50e4]</td>
</tr>
<tr>
<td>r_death_O</td>
<td>% h(^{-1})</td>
<td>Microbial biomass turnover rate in O horizon</td>
<td>[1.0e-4, 1.0e-3]</td>
<td>[7.57e-4, 9.28e-4]</td>
</tr>
<tr>
<td>r_death_A0</td>
<td>% h(^{-1})</td>
<td>Microbial biomass turnover rate in A horizon</td>
<td>[1.0e-4, 1.0e-3]</td>
<td>[3.16e-4, 7.78e-4]</td>
</tr>
<tr>
<td>Vmax_SOC0_O</td>
<td>mg decomposed SOC cm(^{-3}) soil (mg biomass cm(^{-3}) soil(^{-1}) h(^{-1}))</td>
<td>Maximum microbial decomposed SOC in O horizon</td>
<td>[3.0e6, 1.0e9]</td>
<td>[1.85e7, 5.04e7]</td>
</tr>
<tr>
<td>Vmax_SOC0_A0</td>
<td>mg decomposed SOC cm(^{-3}) soil (mg biomass cm(^{-3}) soil(^{-1}) h(^{-1}))</td>
<td>Maximum microbial decomposed SOC in A horizon</td>
<td>[3.0e6, 1.0e9]</td>
<td>[1.45e8, 8.39e8]</td>
</tr>
<tr>
<td>kM_O</td>
<td>mg SOC cm(^{-3}) soil</td>
<td>Half saturation constant in O horizon</td>
<td>[120, 300]</td>
<td>[197.3, 288.5]</td>
</tr>
<tr>
<td>kM_A0</td>
<td>mg SOC cm(^{-3}) soil</td>
<td>Half saturation constant in A horizon</td>
<td>[120, 300]</td>
<td>[160.3, 261.8]</td>
</tr>
<tr>
<td>cuec_O</td>
<td>%</td>
<td>Carbon use efficiency intercept in O horizon</td>
<td>[0.1, 0.9]</td>
<td>[0.38, 0.52]</td>
</tr>
<tr>
<td>cuem_O</td>
<td>% (°C(^{-1}))</td>
<td>Carbon use efficiency temperature slope in O horizon</td>
<td>[-0.03, 0]</td>
<td>[-0.02, -0.01]</td>
</tr>
<tr>
<td>cuec_A0</td>
<td>%</td>
<td>Carbon use efficiency intercept in A horizon</td>
<td>[0.1, 0.9]</td>
<td>[0.48, 0.72]</td>
</tr>
<tr>
<td>cuem_A0</td>
<td>% (°C(^{-1}))</td>
<td>Carbon use efficiency temperature slope in A horizon</td>
<td>[-0.03, 0]</td>
<td>[-0.023, -0.006]</td>
</tr>
</tbody>
</table>
Table 3.4 Parameters priors and 95% CI of posteriors of Q10 model from inverse estimation.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Description</th>
<th>Prior</th>
<th>Posterior 95% CI</th>
</tr>
</thead>
<tbody>
<tr>
<td>kint_O</td>
<td>% h(^{-1})</td>
<td>Intrinsic SOC decomposition rate in O horizon</td>
<td>[1.2e-7, 4.0e-4]</td>
<td>[3.01e-5, 2.02e-4]</td>
</tr>
<tr>
<td>kint_A0</td>
<td>% h(^{-1})</td>
<td>Intrinsic SOC decomposition rate in A horizon</td>
<td>[1.2e-7, 4.0e-4]</td>
<td>[3.9e-5, 9.15e-5]</td>
</tr>
<tr>
<td>theo_O</td>
<td>%</td>
<td>Optimum volumetric soil water content in O horizon</td>
<td>[0.2, 0.9]</td>
<td>[0.32, 0.76]</td>
</tr>
<tr>
<td>theo_A0</td>
<td>%</td>
<td>Optimum volumetric soil water content in A horizon</td>
<td>[0.2, 0.9]</td>
<td>[0.37, 0.5]</td>
</tr>
<tr>
<td>Q10_O</td>
<td>-</td>
<td>Temperature sensitivity of decomposition rate to every 10°C change in temperature in O horizon</td>
<td>[1.0, 5.0]</td>
<td>[1.67, 3.2]</td>
</tr>
<tr>
<td>Q10_A0</td>
<td>-</td>
<td>Temperature sensitivity of decomposition rate to every 10°C change in temperature in A horizon</td>
<td>[1.0, 5.0]</td>
<td>[1.97, 3.3]</td>
</tr>
</tbody>
</table>
C amounts to about 180 g C m$^{-2}$ yr$^{-1}$ and is comparable to data published in other studies (e.g. Zhang et al., 2008). We simulated an increase in litterfall input by 3% every ten years for future projection (Figure 3.2b). The 3% litterfall increase rate (34% increase over 100 years) is chosen as a moderate scenario based on a suite of seven global vegetation models that simulated 34-70% increase in NPP under the HadGEM2-ES RCP 8.5 climate and CO$_2$ scenario [Friend et al., 2014]. We also assumed that a constant fraction of NPP is allocated to litterfall. Litterfall was added to multi-horizon and 3-pool Q10 models according to an exponentially decreasing curve [Fan et al., 2008] (70% to the O horizon and 30% to the A horizon for multi-horizon model; 50%, 30% and 20% for the fast, slow and passive pools of 3-pool Q10 model, respectively). The surface temperature was increased progressively using the Representative Concentration Pathway 8.5 (RCP 8.5) from 2000 to 2100 with a projected overall change of 4.9°C (approximately 0.05 °C yr$^{-1}$ global average) [Arora et al., 2011; Arora et al., 2013]. The scenario we used was a generalized scenario, and was not specific to the region of the field study. Soil moisture values for the warming simulation were based on measurements from the control plot to avoid bias because soil water content in trenched plots is often higher than that of vegetated plots due to lack of transpiration [Hanson et al., 2000]. For the simplicity of the analysis, the projected change in soil moisture in this region was not considered due to its uncertainty under projected warming [Seth et al., 2013].
3.4 Results and Discussion

3.4.1 Inverse estimates of parameters

The model-evaluation statistics showed that all three models can reproduce the field-based estimate of $R_H$ of the trenched plot reasonably well, with an adjusted-$R^2$ ranging from 0.5 to 0.78 for two-horizon models and from 0.58 to 0.80 for one-horizon models (Table 3.5). The root mean squared error (RMSE) of all ensemble runs was highest for the two-horizon ALDA model (0.0023 mg C cm$^{-2}$ h$^{-1}$), and lowest for the one-horizon GERM model (0.0014 mg C cm$^{-2}$ h$^{-1}$). These results support our first hypothesis.

The seasonal dynamics of the modeled soil CO$_2$ flux showed that all seven models could describe the monthly variations in the field-based efflux (Figure 3.3). The two-horizon GERM and ALDA models showed the most divergence among ensemble runs (larger error bar, Figure 3.3a,b), indicating that some of the parameters in these models were poorly constrained. Note that the near-zero winter $R_H$ (Nov-Mar) exhibited in the field-based estimates is best captured by the ALDA model (Figure 3.3a,d).

Whether or not an individual parameter is well constrained can be revealed by its posterior PDF (Figure 3.4; Table 3.6 for parameter descriptions). The posterior PDF of parameters representing SOC intrinsic decomposability (Ea_SOC, activation energy; k) and microbial sensitivity to temperature (Q10, CUE) all exhibited a well-defined unimodal distribution but with different variation. The posterior PDF can also be non-Gaussian distribution in a few cases (e.g. microbial turnover rate in two-horizon GERM model, optimum soil moisture content in two-horizon Q10 model, Figure 3.5-3.6). In general, parameters for the A horizon were less constrained than those for the O horizon as the PDF was relatively flat with large standard deviations. This is likely because the
Table 3.5. Model evaluation statistics from ensemble inverse parameter estimation for three soil models at a deciduous needleleaf forest site. S.D. is the standard deviation of the corresponding metrics from ensemble optimization runs.

<table>
<thead>
<tr>
<th>Model</th>
<th>RMSE (S.D.) (mg C cm(^{-2}) h(^{-1}))</th>
<th>Adjusted-R(^2) (S.D.)</th>
<th>Slope (S.D.)</th>
<th>Intercept (S.D.) (mg C cm(^{-2}) h(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Two-horizon model:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ALDA</td>
<td>0.0023 (0.0003)</td>
<td>0.50 (0.07)</td>
<td>0.84 (0.1) **</td>
<td>0.0031 (0.0003)</td>
</tr>
<tr>
<td>GERM</td>
<td>0.0016 (0.0001)</td>
<td>0.68 (0.02)</td>
<td>0.92 (0.09) **</td>
<td>0.0015 (0.0011)</td>
</tr>
<tr>
<td>Q10</td>
<td>0.0015 (0.00001)</td>
<td>0.78 (0.003)</td>
<td>1.03 (0.02) **</td>
<td>-0.0002 (0.0001)</td>
</tr>
<tr>
<td>One-horizon model:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ALDA</td>
<td>0.0019 (0.0001)</td>
<td>0.58 (0.05)</td>
<td>0.92 (0.1) **</td>
<td>0.0017 (0.0007)</td>
</tr>
<tr>
<td>GERM</td>
<td>0.0014 (0.0001)</td>
<td>0.78 (0.01)</td>
<td>1.15 (0.04) **</td>
<td>-0.0008 (0.0002)</td>
</tr>
<tr>
<td>Q10</td>
<td>0.0015 (4.3e-8)</td>
<td>0.79 (0.001)</td>
<td>1.03 (0.0002) **</td>
<td>-0.0003 (1.9e-6)</td>
</tr>
<tr>
<td>Q10 (3-pool)</td>
<td>0.0017 (2.3e-5)</td>
<td>0.80 (0.005)</td>
<td>1.02 (0.046) **</td>
<td>-0.0001 (0.0003)</td>
</tr>
</tbody>
</table>

**: coefficient is significant at \(p<0.05\)
Figure 3.3 Observed and simulated soil efflux from the three soil decomposition models. Top panel represents the two-horizon versions; bottom panel represents the one-horizon versions. The red lines in (f) represent the results from the 3-pool Q10 model. Error bar shows the uncertainty of simulated CO$_2$ efflux from 100 ensemble runs.
**Table 3.6** Descriptions of a subset of model parameters mentioned in the text.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ea_SOC</td>
<td>J mol$^{-1}$</td>
<td>Activation energy of decomposing SOC to soluble C</td>
</tr>
<tr>
<td>Vmax_SOC0</td>
<td>mg decomposed SOC cm$^{-3}$ soil (mg ENZ cm$^{-3}$ soil)$^{-1}$ h$^{-1}$</td>
<td>Maximum rate of converting SOC to soluble C carbon use efficiency at temperature of 15°C</td>
</tr>
<tr>
<td>CUEc</td>
<td>%</td>
<td>Intrinsic SOC decomposition rate</td>
</tr>
<tr>
<td>k</td>
<td>% h$^{-1}$</td>
<td>Temperature sensitivity of decomposition rate to every 10°C change in temperature</td>
</tr>
</tbody>
</table>
Figure 3.4 Posterior parameter probability density function (PDFs) of three soil decomposition models. The O and A horizon represent the PDFs from the corresponding soil horizon from two-horizon models; one-horizon represents the PDFs from the one-horizon models. Subfigures (g) and (h) represent the results from the 3-pool Q10 model. The range of the x-axis indicates the range of the parameter’s prior uniform distribution.
Figure 3.5 Histograms and kernel fitted probability density functions (PDF, solid red line) show posterior estimates of parameters govern two-horizon ALDA model.
Figure 3.6 Histograms and kernel fitted probability density functions (PDF, solid red line) show posterior estimates of parameters govern two-horizon GERM model.
Figure 3.7 Histograms and kernel fitted probability density functions (PDF, solid red line) show posterior estimates of parameters govern one-horizon Q10 model.
field-based estimate of CO₂ flux is a convolution of both horizons, and the A horizon
likely contributes less to the total flux because of its lower temperature and poorer
substrate quality, thus lacking enough variation (information) to constrain the parameters
for this horizon. Such unsymmetrical informativeness is a common challenge for data
assimilation of multiple horizon decomposition models [Keenan et al., 2012a; Schädel et
al., 2013]. Additional data streams such as incubation data or other pool-specific
measurements may provide the necessary constraints to reduce posterior PDF uncertainty
[Keenan et al., 2012a]. The decomposition rate (k, Figure 3.4g) of the fast SOC pool in
the 3-pool Q10 model was poorly constrained, probably because the small proportion of
light fraction soil makes its CO₂ flux outweighed by that of the slow and passive pools
(0.04-0.14 in Table 3.1, and 0.02-0.1 in posterior distribution of the corresponding
parameter, see Figure 3.7).

Ranges of parameter posterior PDF also reveal characteristics of SOC
decomposition dynamics. The intrinsic decomposability of the A horizon is lower than
that of the O horizon across all two-horizon models (Figure 3.4a,c,e), indicating that C in
deeper soils is more recalcitrant. Deeper soils also had higher Q10, suggesting higher
temperature sensitivity of heterotrophic microorganisms at that depth (Figure 3.4d,f,h), in
line with field experiments from other studies [Lefèvre et al., 2013; Peng et al., 2009;
Zhou et al., 2009]. As expected, the one-horizon model parameters mostly fell within the
mode of the analogous parameters for the O and A horizons in the two-horizon models,
suggesting an averaging effect when lumping heterogeneous soil horizons together. Note
that the CUE in the one-horizon GERM model is notably lower than that of two-horizon
model, suggesting a non-linear interaction structure among parameters (Figure 3.8).
Figure 3.8 Parameter correlation matrix of two-horizon GERM model. * indicates parameter pair that has significant (p<0.05) correlation.
Figure 3.9 Simulated 100 years responses of SOC stock for the three models. Top panel (a-c) is trenched plot simulation; bottom two panels (d-i) are model simulations under 4.8 °C progressive increasing soil temperature and litterfall. The deep blue and red lines (for 3-pool Q10 model) represent ensemble mean from the 100 independent optimization runs for each model, the light colored lines are the results from each ensemble member.
3.4.2 Structural difference induced discrepancy in future SOC stock trajectory

The future projections of the trenched plot differed among the three two-horizon models (Figure 3.9a,b,c). The initial ~5 years SOC stock was similar across all models, where models were constrained by observations and better model-observation matches were achieved. However, the uncertainty in parameter posterior PDF caused diverging responses within each model. Intermodel variation was notable as SOC loss in both microbial models (ALDA and GERM) leveled off after 20 to 40 years, while the Q10 model was still losing C after 100 years. The difference among models was more notable in the litterfall+warming experiments. In the microbial models (ALDA and GERM), the enhanced respiration was compensated by increased litterfall input, so that at the end of 100 years, there was less than 250 mg SOC cm$^{-2}$ difference from the initial SOC stock (Figure 3.9d,e). In contrast, the Q10 model was still losing SOC despite increased litterfall (Figure 3.9f). The overall trend in one-horizon models was similar to that of corresponding two-horizon models, except that both microbial models showed a greater SOC loss around 20 to 40 years (Figure 3.9g,h,i), but this loss was later compensated by increasing litterfall similar to what occurred for the two-horizon models. The 1-pool Q10 model and the ensemble mean of 3-pool Q10 model showed very similar SOC trajectories, although 1-pool Q10 model had much smaller uncertainty range (Figure 3.9i).

Our results demonstrated two different types of uncertainty in decomposition models: (1) uncertainty associated with poorly constrained parameters (i.e., the multiple optima problem) [Brun et al., 2001; Duan et al., 1992]; and (2) the uncertainty associated with conceptual structure of the model (i.e. system identification), which fundamentally relies on our current scientific understanding of the system and its mathematical or numerical
representation. While the first issue may be partially attributed to limitations inherent in the inverse estimation approach, the nonlinear structure of the decomposition model (and any process-based biogeochemical model) also leads to the existence of multiple optima [Duan et al., 1992]. Improved data assimilation techniques may help reduce parameter uncertainty in model calibration and projection [Keenan et al., 2012b; Koffi et al., 2012; Parrish et al., 2012; Zhou et al., 2013], but the uncertainty embedded in model structure (often due to imperfect understanding of the real system) is usually ignored and sometimes difficult to be disclosed by data assimilation alone, as shown in our results.

Detailed examination of various modeled processes help identify key features of different model structures. Both microbial models (ALDA and GERM), either one- or two-horizon, had their labile horizon (O horizon) depleted within the first 20 years (Figure 3.10a,b), and the A horizon to switch from losing C to eventually being a C sink. A similar labile C depletion was exhibited in the 3-pool Q10 model, but not the 2-horizon Q10 model (Figure 3.10c,d), likely because there was not enough information (e.g., an informative prior for decomposition rate) to differentiate the decomposition rate among the two horizons (PDF of decomposition rate of O-horizon is quite flat, indicating high parameter uncertainty, Figure 3.4e). Projected soil R_H also diverged across models, with ALDA and two-horizon GERM models exhibiting a notable initially enhanced R_H upon warming for about 5 years and then stabilized at a similar level (Figure 3.11a,b,d), although the ALDA model has a much larger oscillation in soil R_H due to the same oscillation in microbial biomass (Figure 3.12a). Overall, for the depletion of labile C, warming enhanced R_H and loss of SOC, which was later attenuated, and SOC loss
Figure 3.10 Simulated 100 years responses of SOC stock for each of the horizons for the 2-horizon models and 3-pool Q10 model. The deep blue and red lines (for 3-pool Q10 model) represent ensemble mean from the 100 independent optimization runs for each model, the light colored lines are the results from each ensemble member.
Figure 3.11 Simulated 100 years soil $R_{\text{H}}$ for the three models. The deep blue and red lines (for 3-pool Q10 model) represent ensemble mean from the 100 independent optimization runs for each model, the light colored lines are the results from each ensemble member.
Figure 3.12 Microbial biomass C (a,b,a1,b1) and CUE (c,d,c1,d1) changes in the ALDA and the GERM models (two-horizon and one-horizon) under warming plus litterfall model simulations. Annual microbial biomass and 30-day moving average of hourly CUE are shown in a-d; seasonal microbial biomass and CUE dynamics for the first 5 years are shown in embedded graph a1-d1.
eventually being compensated by increased litterfall of ALDA and GERM model matched the observed C dynamics in long-term soil warming experiments [Kirschbaum, 2004; Knorr et al., 2005; Luo et al., 2001; Melillo et al., 2011]. Despite the oscillatory behavior of microbial models which may be improved by multi-pool representations (especially ALDA, see discussion of oscillation in Section 3.4.3), their future projections matched better with observations than the conventional Q10 models, supporting our second hypothesis. Site-level parameterization of microbial decomposition models probably requires more measurements to be able to constrain parameters well (under-parameterized, tend to have high biases), while a simple Q10 type of model is likely to be over-parameterized (high variance) with good calibration results but may fail when tested under different scenarios.

There are several limitations of this study that need to be explored further to make the results more generally applicable. First, our hierarchy of models was applied to a limited dataset which is specific to a particular ecosystem and soil type. A more comprehensive study that covers various ecosystems and soil properties would help to separate ecosystem-specific recommendations for model selection from more generalized conclusions. Second, this limited dataset also imposes a certain structure on our model in that the 2-horizon model is composed of O and A horizons for the larch forest we tested. Models should be conceptually tailored to match the ecosystem characteristics being simulated. If the models were to be applied in a grassland ecosystem, which generally does not possess an O horizon, then a one-horizon model or a multi-layer model with parameters that correspond to observed depth-resolved decomposition properties may be appropriate. Third, we assumed constant soil moisture for future scenarios and did not
include a feedback of soil moisture to soil temperature. This feedback could result in a
different SOC trajectory than what we presented, yet the divergent model response
probably would still exist due to the model structures. Fourth, in our long-term
extrapolation, an implicit assumption was that the model structure and represented
processes are appropriate for the simulation period. Such an assumption is debatable. An
option to address model structural uncertainty is Bayesian model averaging where a
dynamic range of model structures are weighted by their posterior model probability
[Hoeting et al., 1999; Wasserman, 2000].

We also acknowledge that we are limited to only 4-years of observations to
inform the model, and that a longer period of observation (decadal to multi-decadal)
would have provided tighter constraints. This is especially true given the slow turnover
rate of SOC. The importance and difficulty of constraining parameters associated with
slow decomposition processes was also recognized in a twelve-year study in a temperate
deciduous forest in the Eastern U.S. [Braswell et al., 2005]. For an efficient assimilation,
data length is only one aspect, data quality and the amount of information encompassed
by the observation is also critical [Liu and Gupta, 2007]. We argue that from the
perspective of efficient data assimilation, other characteristics of the soil system (e.g.
microbial related features) can help identify proper parameters that will constrain the
modeling system and thus should be included in the model. Note however that because
the Q10 model has only one variable (i.e. SOC stock) that can be evaluated, the increased
availability of other soil related data (e.g. measured CUE, MIC pool sizes [Frey et al.,
2013; Serna-Chavez et al., 2013]) cannot further inform the Q10 model. Without the
support of sufficiently long and diverse observations to inform the model, model
structure becomes a dominating factor in the future projection of SOC. It is worthy to note here that under the warming plus litterfall scenario, the trajectories of the three models can differ notably from each other. Therefore, observations from warming manipulations or other manipulating experiments would be very valuable for informing models, as parameters should be better constrained.

### 3.4.3 Structural difference induced discrepancy in microbial activity

In this study, different conceptual structures of microbial models led to different response trajectories. Annual average microbial biomass in both the ALDA and GERM models exhibited an initial increase and leveled off around year 60 and year 40 respectively (Figure 3.12a,b). Oscillatory behavior of microbial models has been analytically demonstrated by Wang et al. [2013], and is exhibited in the interannual variation of MIC of the two models in this study. The amplitude is much greater in the ALDA model, which is likely caused by the sensitivity of microbial biomass to soil moisture variation in the model (Pearson correlation between MIC and soil moisture is 0.6, p<0.05), a sensitivity that does not occur in GERM model as soil moisture was not represented. In our field measurements, soil moisture increased in the 2nd and 3rd year and then slightly declined in subsequent years, such interannual cyclic moisture variation drove the MIC response so that MIC tightly tracked the moisture in the ALDA model. The increased MIC at the beginning of the simulation likely reflects the microbial responses to existing root exudates and sloughed-off cells that cannot be accounted for by correcting measured CO₂ efflux using root biomass. The high sensitivity of microbial activity to rhizodeposition (or so called “rhizosphere priming effect”, Kuzyakov, 2002) suggests that microbial models should account for the interaction between root and
microbial activity. The seasonal patterns of MIC in both models were similar with both featuring lower MIC during the growing season and accumulating during the winter (Figure 3.12a1,b1). This agreed well with the previously reported observed seasonal dynamics of soil microbial biomass C for the same site [S Liu and Wang, 2010].

The dynamics of CUE were also different between the two models, despite the similar seasonal dynamics where lower CUE occurs during the growing season than during the non-growing season. Because the GERM model used prescribed CUE as a linearly decreasing function of temperature, CUE decreased consistently due to progressive warming (Figure 3.12d). In contrast, in the modified ALDA model, CUE was simulated as a function of the ratio between respired CO₂ and assimilated SOC, which were both explicitly controlled by environmental conditions. Therefore, CUE of the ALDA model did not vary much with temperature (Figure 3.12c). Note that the upward shift in CUE in ALDA model around year 20 is caused by a depletion of the O horizon due to fast substrate assimilation (Figure 3.10a), in line with Knorr et al. [2005] and Kirschbaum [2004] where their modeling approaches suggested “substrate depletion” as an explanation for apparent thermal acclimation in soil respiration under warming climate. Given the fairly good inverse estimation results against field-based estimates of both models, we conclude that both changing and constant CUE are plausible with increasing temperature. Note that the average MIC declined in the ALDA 2-horizon model under warming scenario (Figure 3.12a) yet CUE increased due to depletion of O-horizon. This is because the activation energy that controls SOC enzymatic decay of A horizon is smaller than that of microbial respiration (Figure SI 2, Ea_SOC_A0 < Ea_Sx_A0)
indicating smaller temperature sensitivity, therefore, the amount of Soluble C (substrate) consumed relative to microbial biomass declined with warming.

It is worth noting here that the oscillation amplitude of microbial biomass in the two-horizon ALDA model is notably smaller than that of the one-horizon model, which may be due to a more heterogeneous architecture of the soil C pools. The oscillations arise because of tight coupling between microbial and SOC pools, yet this behavior might weaken with greater pool heterogeneity in microbial models. In reality, there are many organisms consuming chemically heterogeneous substrates on varying timescales. Such heterogeneity could dampen the oscillations.

It should also be acknowledged that we tested a simplified modeling framework because the decomposition model was not coupled to other key element cycles. Soil C sequestration under ambient and rising atmospheric CO$_2$ can be constrained directly by nitrogen availability and indirectly by nutrients that supports N$_2$ fixation [Hobbie et al., 2002; van Groenigen et al., 2006]. Kinetic and stoichiometric constrains on microbial physiology also pose key controls over SOC decomposition dynamics [Allison, 2005; Sinsabaugh et al., 2013]. Incorporating those interactions into models could produce even more realistic future SOC dynamics than the models used in this study.

### 3.5 Conclusion

In this study, we calibrated three structurally different soil organic matter decomposition models (Q10 and two microbial models with different complexities) against in-situ soil efflux observations, each with two-horizon and one-horizon versions. The calibration and validation results showed that all models can reasonably simulate four years of field-based estimates of R$_H$ from a forest plot. However, there were
differences among the models’ projected decomposition dynamics under increased
temperature and litterfall. Our study has three main conclusions. First, effective
parameters estimation requires sufficient data length and information content. For soils
with long turnover time, long period of observations and multiple data streams (e.g.,
microbial biomass, enzyme characteristics) are needed to adequately constrain the models.
Second, conceptual understanding of the ecological mechanisms represented in models
dominates the trajectory of model projections among models that assimilate the same data
to constrain parameters. While all the models in our study produced similar
decomposition dynamics early in the projected simulations, the long-term projections
varied substantially across all models. This indicates that there is substantial uncertainty
associated with microbial processes among the models. Finally, labile C depletion was
observed in both two-horizon microbial models. The substrate depletion shifted the
carbon use efficiency in the ALDA model to result in an efficiency level and SOC
trajectory similar to that of the GERM model in which carbon use efficiency was
prescribed to decline with increasing temperature. This suggests that both constant or
variable carbon use efficiency are plausible when modeling future decomposition
dynamics, and that short-term (e.g. a few years) observations are not sufficient to inform
model parameters of the long-term responses of microbial thermal adaption.

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CHAPTER 4. INCORPORATING MICROBIAL DORMANCY DYNAMICS INTO SOIL DECOMPOSITION MODELS TO IMPROVE QUANTIFICATION OF SOIL CARBON DYNAMICS AND MICROBIAL BIOMASS OF GLOBAL TEMPERATE FOREST ECOSYSTEMS

4.1 Abstract

Soil carbon (C) feedbacks to climate change result from responses of plant and microbial communities and nutrient cycling to environmental changes. Explicit consideration of microbial life history traits and strategy may be necessary to predict climate feedbacks due to microbial physiology and community changes and their associated effects on C cycling. In this study, we developed an explicit microbial-enzyme decomposition model and examined model performance with and without representation of microbial dormancy across 6 temperate forest sites representing different forest types. The dormancy model consistently produced a better match with field observed heterotrophic soil CO$_2$ efflux ($R_H$) in comparison with the no-dormancy model, which exhibited larger seasonal oscillation and overestimation in microbial biomass. Our regional modeling results further indicated that models with dormancy were able to produce more realistic magnitude in microbial biomass and soil $R_H$. Spatial correlation analysis showed that soil organic C content was the dominating factor in the simulated

He, Y., J. Yang, Q. Zhuang, J. W. Harden, A. D. McGuire, Y. Liu, G. Wang. Incorporating microbial dormancy dynamics into soil decomposition models to improve quantification of soil carbon dynamics and microbial biomass of global temperate forest ecosystems I. To be submitted.
spatial pattern of soil $R_H$ in both models, suggesting that Michaelis-Menten kinetics may not be appropriate for models that do not vertically resolve decomposition dynamics in the soil profile. In contrast to strong temporal and local controls of soil temperature and moisture on microbial dormancy, soil carbon-to-nitrogen ratio (C:N) was a major regulating factor at regional scales, indicating scale-dependent biogeochemical controls on microbial dynamics. Our findings suggest that incorporating microbial dormancy could improve the realism of microbial-based decomposition models. The use of mechanistic approaches in soil decomposition models enhances the avenues for integration of empirical soil experiments and modeling.

4.2 Introduction

Soil has always been a focus of climate change studies due to its large carbon (C) stocks – the global soil organic C (SOC) stock is at least four times greater than atmospheric C [Jobbágy and Jackson, 2000] and soil respiration is the second largest flux between the biosphere and the atmosphere following photosynthesis [Raich and Potter, 1995]. Therefore soil C dynamics play a key role in net C sequestration of terrestrial ecosystems and is essential to our understanding of biogeochemical cycles and its climate-C interactions [IPCC, 2013].

Since there are limitations of traditional first-order decomposition modeling approach in current earth system models [Todd-Brown et al., 2013], microbial-based soil organic matter decomposition models have been increasingly used in recent studies at both site and global scales [Allison et al., 2010; He et al., 2014a; Wieder et al., 2013]. The current generation of microbial-based decomposition models usually features a common framework where enzyme production and microbial physiology are associated
with total microbial biomass (MIC), which has a direct coupling with SOC enzymatic decomposition. A key microbial life-history trait that is usually lacking in these models is microbial dormancy. Dormancy is a common, bet-hedging strategy used by microorganisms when environmental conditions limit growth and reproduction [Jones and Lennon, 2010; Lennon and Jones, 2011]. When microorganisms are confronted with unfavorable conditions, they may enter a reversible state of low metabolic activity and resuscitate when favorable conditions occur. Microorganisms in this state of reduced metabolic activity are not able to drive biogeochemical processes such as soil CO$_2$ production; therefore only active microorganisms are involved in utilizing substrates in soils [Blagodatskaya and Kuzyakov, 2013]. Although there are some studies which have explicitly incorporated dormancy into models [Ayati, 2012; S Blagodatsky and Richter, 1998; Panikov and Sizova, 1996; Wang et al., 2014b; Wirtz, 2003], they are mostly confined to incubation experiments, and applications of microbial models generally do not consider dormancy.

The representation of dormancy in microbial-based decomposition models may be necessary due to several main motivations that led to the inception of this study: (1) current coupled SOC-MIC structure leads to oscillatory behavior of both pools with unrealistically large amplitudes of interannual variation [Wang et al., 2013; Wieder et al., 2013], thus incorporating dormancy may structurally improve model realism; (2) there is a scale mismatch among common measurement procedures of microbial biomass–based physiological metrics. For example, substrate induced respiration and fumigation techniques measure the total microbial biomass when conversion factor 40.04 calculated by [Anderson and Domsch, 1978] is used, whereas Phospholipid Fatty Acid (PLFA) and
fluorescence in situ hybridization (FISH) measure the active proportion of total biomass [Blagodatskaya and Kuzyakov, 2013; Denef et al., 2009; Kramer and Gleixner, 2006]; (3) the aforementioned inconsistency may pose challenges in data-model integration and in microbial model comparisons and evaluation; (4) the transition between dormant and active state of microbes can be fast (in the order of hours to days) with substantial magnitude change (e.g., an order of magnitude) in the proportion of active biomass and relative abundance of different phylogenetically clustered microbial groups, but with little changes in total microbial biomass [Blagodatsky et al., 2000; Hagerty et al., 2014; Placella et al., 2012].

In this study, we hypothesize that: (1) a microbial model incorporated with dormancy would outperform the model without dormancy at site-level parameterization; and (2) a microbial model with dormancy would produce more realistic microbial biomass and soil R_H on both site-level and regional scales. We compared two microbial models, that with and without representation of dormancy, for site and regional patterns of the modeled SOC and microbial related variables. We also discussed the primary controls on microbial and SOC dynamics at different tempo-spatial scales.

4.3 Methods

4.3.1 Model description

Dormancy was incorporated into an existing microbial-enzyme conceptual framework described by Allison et al. [2010], in which an Arrhenius formulation of temperature sensitivity was replaced with a simplified temperature sensitive Q_{10} function \( Q_{10}^{\text{temp} - 15} \) to reduce the number of model parameters. The reversible transition between
dormant and active state of microbial biomass is assumed to be controlled by environmental cues – directly accessible substrates, as demonstrated in Wang et al. [2014a]. We integrate Davidson et al.’s [2012] conceptual framework of quantifying concentration of soluble C substrates that are directly accessible for microbial assimilation, thus building a direct linkage between environmental factors with microbial state transitions. Substrate quality is also reflected in the model through a generic index of soil C:N ratio [Manzoni et al., 2008] and the assimilation of substrate by microorganisms is assumed to be regulated by the C:N ratio of microbial biomass and that of the soil. The model simulates the microbial and SOC dynamics for the top 30cm of the soil column. The equations for the model with microbial dormancy are as follows:

\[
\frac{dSOC}{dt} = \text{Input} - V_{\text{max}} Q_{\text{10enz}}^{\text{10}} ENZ \left( \frac{SOC}{K_m + SOC} \right) (120 - CN) \tag{4.1}
\]

\[
\frac{d\text{SolubleC}}{dt} = \text{Decomposition} - \frac{1}{Y_g \alpha} m_{\text{R}} Q_{\text{10mic}}^{10} B_a \left( \frac{CN_{\text{soil}}}{CN_{\text{mic}}} \right)^{0.6} + B_a r_{\text{death}} + ENZ r_{\text{loss}} \tag{4.2}
\]

\[
\frac{dB_a}{dt} = \left( \frac{\phi}{\alpha} - 1 \right) m_{\text{R}} Q_{\text{10mic}}^{10} B_a \left( \frac{CN_{\text{soil}}}{CN_{\text{mic}}} \right)^{0.6} - (1 - \phi) m_{\text{R}} Q_{\text{10mic}}^{10} B_a + \phi m_{\text{R}} Q_{\text{10mic}}^{10} B_d - B_a r_{\text{prod}} - B_a r_{\text{death}} \tag{4.3}
\]

\[
\frac{dB_d}{dt} = -\beta m_{\text{R}} Q_{\text{10mic}}^{10} B_d + (1 - \phi) m_{\text{R}} Q_{\text{10mic}}^{10} B_a - \phi m_{\text{R}} Q_{\text{10mic}}^{10} B_d \tag{4.4}
\]

\[
\frac{dENZ}{dt} = B_a r_{\text{prod}} - ENZ r_{\text{loss}} \tag{4.5}
\]

where state variables are SOC, SolubleC, B_a, B_d and ENZ, corresponding to SOC content, SolubleC content, microbial biomass in active and dormant state respectively, and
enzyme C (mgC cm\(^{-2}\)); temp is soil temperature at each time step \(t\); \(\phi\) is directly accessible substrate for microbial assimilation, calculated based on Michaelis-Menten kinetics formulated as 
\[
\phi = \frac{SolubleC \times D_{\text{liq}} \times \theta^3}{K_s + SolubleC \times D_{\text{liq}} \times \theta^3},
\]
where \(D_{\text{liq}}\) is a diffusion coefficient of the substrate in liquid phase (determined by assuming all soluble substrate is directly accessible at the reaction site, formulated as 
\[
D_{\text{liq}} = \frac{1}{(1 - BD / PD)^3};
\]
BD is bulk density and PD is soil particle density); \(\theta\) is volumetric soil moisture content, and \(K_s\) is corresponding Michaelis constant \([Davidson et al., 2012]\). Detailed description for other parameters is summarized in Table 4.1. Adding up the equation 3 and 4 shown above gives the model without dormancy.

Environmental factors such as substrate availability are often thought to be a direct control of the transition between active and dormant states of microorganisms \([Lennon and Jones, 2011]\). Therefore we adopted the formulation described in \(Wang et al., [2014a]\), where the transition between active and dormant state of microorganisms is scaled linearly with substrate availability and the direction of the net transition is determined by the balance of maintenance metabolic requirement and substrate availability.

We recognize that our model only simulates C dynamics, and decomposition is effectively influenced by various nutrients through kinetic and stoichiometric constrains that are not explicitly represented in this model \([Allison, 2005; Hobbie et al., 2002; Sinsabaugh et al., 2013; van Groenigen et al., 2006]\). Instead of using a more sophisticated modeling framework, we introduced a temperature and population size
dependent scaling factor on the potential microbial death rate, formulated as

\[ 1.5^{\frac{temp-15}{10}} \times \frac{B_d}{SOC \times 0.025} \]

where a metabolic temperature sensitivity of 1.5 and a population capacity of 2.5% of SOC is assumed for temperate forest soils [Xu et al., 2013; Yvon-Durocher et al., 2012]. This multiplier is used to modify the parameter \( r_{\text{death}} \) and implicitly represents competition for nutrients and down regulates microbial growth.

4.3.2 Model calibration and validation

We calibrated the model at 6 different temperate forest sites in northeastern China (3) and contiguous USA (3) with a latitudinal span of 38 – 45°N using a global optimization algorithm known as the SCE-UA (shuffled complex evolution; [Duan et al., 1992; Duan et al., 1994]) (Table 4.2). The 3 northeastern China sites were all trenched plots with monthly measured \( R_H \), soil temperature and gravimetric soil moisture content at 10cm from 2004 to 2007 [Wang and Yang, 2007; Wang et al., 2006]. The 3 US sites are part of the AmeriFlux network. The level 2 (gap-filled) eddy covariance data with half-hourly measured soil temperature (at 10cm, °C), volumetric soil moisture content (at 10cm, %; VSM) and automated soil chamber measured soil respiration (umol m\(^{-2}\) s\(^{-1}\)) were used for this study [Gu et al., 2006; Irvine and Law, 2002]. Approximately 50% of soil respiration was assumed to be \( R_H \) [Hanson et al., 2000]. Litterfall was assumed to be a fixed proportion (0.3) of net primary production (NPP), and we assume NPP/GPP = 0.45 (gross primary production, GPP) [Law et al., 2001; Law et al., 2003]. GPP at US-Me2 and US-MRf sites (see Table 4.2) were also obtained from level 2 data, but were not available for the US-MOz site. Therefore for the \( R_H \) measurement period (2004-2007), we used level 4 gap-filled net ecosystem exchange (NEE) and we calculated GPP based
on NEE and meteorological data using an online flux partitioning tool (http://www.bgc-jena.mpg.de/~MDIwork/eddyproc/upload.php) [Lasslop et al., 2010]. Site level state variables (e.g. SOC content) served as initial states for the model calibration. Note that we rescaled the prior used in inverse modeling for parameters on per unit of microbial biomass basis (Table 4.1). The first 75% of total available data at each site was used for calibration and the remaining was used for validation. Model evaluation statistics were calculated using the whole data series.

4.3.3 Data sources for spatial extrapolation

We used the above calibrated ecosystem specific parameters and extrapolated to the whole temperate forest region defined as the latitudinal band from 25°N to 50° N. We did not include the Southern Hemisphere due to limited forest coverage and lack of calibration sites located in the region. The average parameters of the corresponding forest types are used for each forest type involved the latitudinal band. Forest land cover information was extracted from Moderate Resolution Imaging Spectroradiometer (MODIS) land cover product (MCD12C1) for the period 2000-2012 and annual mean land cover distribution was used. The original 0.05°×0.05° (lon×lat) resolution grid was aggregated to 0.5°×0.5° using a majority resampling approach to best preserve the spatial structure of the major classes. NPP (2000-2012, annual mean) data were extracted from the MOD17A3 L4 Global 1km product (Version-55) [Zhao and Running, 2010]. The original data were aggregated to 0.5°×0.5° using the areal mean. Soil physical properties and organic C and N content of the top 30cm were obtained from gridded Global Soil Dataset for use in Earth System Models (GSDE) dataset [Shangguan et al., 2014].
Table 4.1 Calibration sites that are used in this study, including 3 sites from northeastern China and 3 AmeriFlux sites from the coterminous USA. Soil properties are based on the total element content or measurements in the top 30 cm of soil.

<table>
<thead>
<tr>
<th></th>
<th>Mixed deciduous forest (CN-Mixed)</th>
<th>Oak forest (CN-Oak)</th>
<th>Larch plantation (CN-Lar)</th>
<th>Marys River Fir (US-MRF)</th>
<th>Metolius Intermediate Pine (US-Me2)</th>
<th>Missouri Ozark (US-MOz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude, longitude</td>
<td>45.33-45.42N, 127.50-127.56E</td>
<td>45.33-45.42N, 127.50-127.56E</td>
<td>45.33-45.42N, 127.50-127.56E</td>
<td>44.65N, 123.55W</td>
<td>44.45N, 121.56W</td>
<td>38.74N, 92.20W</td>
</tr>
<tr>
<td>Elevation (masl)</td>
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<td>400</td>
<td>400</td>
<td>263</td>
<td>1253</td>
<td>219</td>
</tr>
<tr>
<td>MAT, MAP</td>
<td>2.8°C, 700cm</td>
<td>2.8°C, 700cm</td>
<td>2.8°C, 700cm</td>
<td>9.0°C, 1350mm</td>
<td>10°C, 480mm</td>
<td>12.8°C, 940mm</td>
</tr>
<tr>
<td>Vegetation (IGBP)</td>
<td>Mixed forest</td>
<td>Deciduous broadleaf forest</td>
<td>Deciduous needleleaf forest</td>
<td>Evergreen needleleaf forest</td>
<td>Evergreen needleleaf forest</td>
<td>Deciduous broadleaf forest</td>
</tr>
<tr>
<td>Soil type</td>
<td>Sandy loam</td>
<td>Sandy loam</td>
<td>Sandy loam</td>
<td>Sandy loam*</td>
<td>Sandy loam</td>
<td>Silt loam</td>
</tr>
<tr>
<td>Clay %</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>7</td>
<td>-</td>
</tr>
<tr>
<td>Sand %</td>
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<td>-</td>
<td>-</td>
<td>-</td>
<td>67</td>
<td>-</td>
</tr>
<tr>
<td>Silt %</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>26</td>
<td>-</td>
</tr>
<tr>
<td>Soil C:N</td>
<td>13.6</td>
<td>20.6</td>
<td>15.8</td>
<td>23.86 *</td>
<td>23.86</td>
<td>16 *</td>
</tr>
<tr>
<td>SOC fraction (%)</td>
<td>9.7</td>
<td>7.6</td>
<td>4.8</td>
<td>1.2 *</td>
<td>1.2</td>
<td>8 *</td>
</tr>
<tr>
<td>Bulk density (g cm⁻³)</td>
<td>0.63</td>
<td>0.58</td>
<td>1.01</td>
<td>1.15 *</td>
<td>1.15</td>
<td>1.37</td>
</tr>
<tr>
<td>Microbial biomass C</td>
<td>1950</td>
<td>1050</td>
<td>900</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>(mg kg⁻¹)⁶</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Microbial biomass N (mg kg⁻¹)⁶</td>
<td>210</td>
<td>110</td>
<td>90</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Microbial C:N⁶</td>
<td>9.3</td>
<td>9.6</td>
<td>10</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>MIC/SOC⁶</td>
<td>0.013</td>
<td>0.011</td>
<td>0.009</td>
<td>0.016</td>
<td>0.016</td>
<td>0.99</td>
</tr>
</tbody>
</table>

|---|---|---|---|---|---|---|

* Values are not reported in literature, average of the same ecosystem type are used for substitution.
Table 4.2 Description of parameters used in the model and the prior used in inverse modeling. The value is given if parameter is predefined to be a constant and is not used in inverse modeling. Parameters that are per microbial biomass based have different priors for dormancy and no-dormancy model. Note that the model simulates top 30 cm of soil.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Prior / value (Dormancy model)</th>
<th>Prior / value (No-Dormancy model)</th>
<th>Notes and citations</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>Maintenance respiration weight, $m_R/(\mu_G+m_R)$, where $\mu_G$ is specific growth rate (h⁻¹)</td>
<td>[0.01, 0.5]</td>
<td>[0.005, 0.05]</td>
<td>[Wang et al., 2014]</td>
</tr>
<tr>
<td>β</td>
<td>Ratio of dormant microbial maintenance rate to $m_R$</td>
<td>[0.0005, 0.005]</td>
<td>-</td>
<td>[Wang et al., 2014]; [Blagodatskaya and Kuzyakov, 2013]</td>
</tr>
<tr>
<td>$m_R$</td>
<td>Specific maintenance rate for active biomass (h⁻¹)</td>
<td>[0.001, 0.08]</td>
<td>[0.0001, 0.008]</td>
<td>[Wang et al., 2014]; [Schimel and Weintraub, 2003]; [Blagodatskaya and Kuzyakov, 2013]</td>
</tr>
<tr>
<td>Ks</td>
<td>Half-saturation constant for directly accessible substrate (mgC cm⁻²)</td>
<td>[0.01, 10]</td>
<td>Same</td>
<td>Calculated based on approximate range of SolubleC/SOC ratio of 1e⁻⁴–1e⁻³ [Davidson et al., 2012a] and reported Ks for substrate breakdown of 72mg kg⁻¹ soil [Xu et al., 2014]</td>
</tr>
<tr>
<td>Km</td>
<td>Half-saturation constant for enzymatic decay of SOC (mgC cm⁻²)</td>
<td>[200, 1000]*</td>
<td>Same</td>
<td>Assuming SOC is not at saturation for enzymatic decay [Schimel and Weintraub, 2003]</td>
</tr>
<tr>
<td>Vmax</td>
<td>Maximum SOC decay rate</td>
<td>[1e⁻⁴, 5e⁻³]</td>
<td>Same</td>
<td>Calculated based on the magnitude of litter input C</td>
</tr>
</tbody>
</table>
| r_prod    | Enzyme production rate of active microorganism (h⁻¹)                        | [1e⁻⁴, 8e⁻⁴]                   | [1e⁻⁵, 8e⁻⁵]                     | [Schimel and Weintraub, 2003] assumes 5% of the C uptake by microorganism is allocated to exoenzymes production (d⁻¹). This is equivalent to an hourly rate of 2e⁻³ h⁻¹; the
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>r_loss</td>
<td>Enzyme loss rate (h⁻¹)</td>
<td>[0.0005,0.002]</td>
<td>Same [Allison et al., 2010]; [Schimel and Weber, 2003]</td>
</tr>
<tr>
<td>r_death</td>
<td>Potential rate of microbial death (h⁻¹)</td>
<td>[2e⁻⁴, 2e⁻³]</td>
<td>[Allison et al., 2010]; [Xu et al., 2014];</td>
</tr>
<tr>
<td>Q10_enz</td>
<td>Temperature effects on enzyme activity (rate change per 10°C increase in temperature). Based on 6% rate increase per °C.</td>
<td>1.79</td>
<td>Same [Purich, 1996]</td>
</tr>
<tr>
<td>Q10_mic</td>
<td>Temperature effects on microbial metabolic activity (rate change per 10°C increase in temperature). Based on 0.65eV activation energy for soils.</td>
<td>[1.5, 3.5]</td>
<td>Same [Yvon-Durocher et al., 2012]</td>
</tr>
<tr>
<td>Yg</td>
<td>True growth yield, or carbon use efficiency</td>
<td>[0.3, 0.7]</td>
<td>Same [Sinsabaugh et al., 2013]</td>
</tr>
<tr>
<td>Yg_slope</td>
<td>Temperature sensitivity of Yg per °C increase</td>
<td>-0.012</td>
<td>Same [German et al., 2012]</td>
</tr>
<tr>
<td>Initial active fraction (r₀)</td>
<td>Active proportion of microbial biomass</td>
<td>[0.05, 0.3]</td>
<td>- [Lennon and Jones, 2011]</td>
</tr>
</tbody>
</table>

* Upper bound of 2500 is used for US-MOz due to its high SOC content.
density was calculated based on bulk density and porosity, and porosity was estimated using VSM at -10kPa (provided in GSDE). Specifically, we assumed saturated VSM as same as VSM at -10kPa for silt loam soil and we added 10% for sand loam soil based on the soil water retention curve [Cornelis et al., 2005]. Soil was classified according to soil taxonomy [Soil Survey Staff, 2003] and using sand, silt, and clay content from the GSDE data set. For transient simulations, we used CMIP5 historical runs initialized in year 2006 from CCSM4 land modeling realm (r1i1p1) to retrieve soil temperature (tsl, average of top 10cm) and soil water content in the top 10cm (mrsos) (http://www.earthsystemgrid.org). Soil water content in mass was converted to soil volumetric moisture using relevant soil properties provided by the GSDE dataset. Soil temperature and moisture data were interpolated from 0.9° × 1.25° to 0.5° × 0.5° using bilinear interpolation method [Wang et al., 2006].

4.3.4 Statistical Analysis

Because we are interested in the overall functional correlations between dormancy and related environmental factors, we choose to use simple Pearson correlation for spatial correlation analysis. The spatial extrapolation used the soil temperature and moisture profile from 2006 and the model was run for 3 years. The simulation results for the last year were used for spatial grid-based and temporal correlation analysis.

4.4 Results

4.4.1 Site level calibration and validation

Both the dormancy and no-dormancy models can reproduce the observed soil R_H reasonably well. The dormancy model across the six sites showed adj-R^2 ranging from 0.50 to 0.76 (Table 4.3), with Nash-Sutcliffe model efficiency coefficients of similar
range (0.49 to 0.75). The no-dormancy model performed notably worse in five out of the six sites (except US-MRf site) as adj-$R^2$ ranged from 0.12 to 0.58; the Nash-Sutcliffe coefficients were also much lower and were even negative at three sites (Table 4.3). The no-dormancy model did not adequately reproduce the observed soil respiration well at Missouri Ozark AmeriFlux site (US-MOz) (adj-$R^2 = 0.12$), likely because the high SOC content at this site makes it more difficult to find an appropriate $K_m$ due to its high sensitivity (see discussion in Section 4.4.3). A paired t-test on root mean square error, adj-$R^2$ and Nash coefficient showed significant differences between the two models (df=5; $p<0.05$ for RMSE; $p<0.01$ for adj-$R^2$; and $p<0.05$ for Nash coefficient). Simulated dynamics of various C pools (e.g., SOC, SolubleC, ENZ and MIC) of the two models exhibited similar patterns over time (Figure 4.1, 4.2). SOC at US-Me2 showed a slight decline over the course of 11 years in both models (Figure 4.1a,e), with SolubleC content showing a seasonal fluctuation anti-phased with microbial biomass due to active substrate uptake during summer thus less substrate availability, and suppressed microbial activity during winter, which led to the accumulation of substrate (Figure 4.1a,e). The active proportion of microbial biomass tracked the changes in soil moisture tightly, despite the opposite moisture regimes at the two sites where US-Me2 experienced moderate drought during summer while CN-Lar featured benign moisture conditions for microbial decomposition (Figure 4.1b,f; Figure 4.2b,f). It is worth noting here that the seasonal MIC amplitude (calculated as the difference between annual maximum and minimum MIC) was always much larger (up to two times larger) in no-dormancy models than in the dormancy models (Table 4.3; Figure 4.1b,g; Figure 4.2b,g), and there was significant
Table 4.3 Model evaluation statistics from ensemble inverse parameter estimation for dormancy and no-dormancy model at the 6 temperate forest sites. NS is the Nash-Sutcliffe model efficiency coefficient. The significance of the difference of metrics between the two models is tested using paired t-test.

<table>
<thead>
<tr>
<th>Model</th>
<th>RMSE (S.D.)** (mg C cm⁻² h⁻¹)</th>
<th>Adjusted-R² (S.D.***</th>
<th>NS coefficient**</th>
<th>Seasonal MIC amplitude (mg C cm⁻²)**</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Dormancy model:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CN-Mixed</td>
<td>0.0037</td>
<td>0.58</td>
<td>0.54</td>
<td>2.82</td>
</tr>
<tr>
<td>CN-Oak</td>
<td>0.0030</td>
<td>0.73</td>
<td>0.72</td>
<td>0.92</td>
</tr>
<tr>
<td>CN-Lar</td>
<td>0.0017</td>
<td>0.74</td>
<td>0.72</td>
<td>0.68</td>
</tr>
<tr>
<td>US-MRf</td>
<td>0.0011</td>
<td>0.76</td>
<td>0.75</td>
<td>1.72</td>
</tr>
<tr>
<td>US-Me2</td>
<td>0.0011</td>
<td>0.66</td>
<td>0.63</td>
<td>1.97</td>
</tr>
<tr>
<td>US-MOz</td>
<td>0.0017</td>
<td>0.50</td>
<td>0.49</td>
<td>1.10</td>
</tr>
<tr>
<td><strong>No-dormancy model:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CN-Mixed</td>
<td>0.0080</td>
<td>0.29</td>
<td>-1.39</td>
<td>5.79</td>
</tr>
<tr>
<td>CN-Oak</td>
<td>0.0044</td>
<td>0.38</td>
<td>-1.13</td>
<td>6.68</td>
</tr>
<tr>
<td>CN-Lar</td>
<td>0.0031</td>
<td>0.49</td>
<td>0.32</td>
<td>7.60</td>
</tr>
<tr>
<td>US-MRf</td>
<td>0.0009</td>
<td>0.70</td>
<td>0.69</td>
<td>2.39</td>
</tr>
<tr>
<td>US-Me2</td>
<td>0.0019</td>
<td>0.58</td>
<td>0.29</td>
<td>3.60</td>
</tr>
<tr>
<td>US-MOz</td>
<td>0.0044</td>
<td>0.12</td>
<td>-2.3</td>
<td>2.50</td>
</tr>
</tbody>
</table>

Metrics are significantly different at p<0.1; ** p<0.05; *** p<0.01;
Figure 4.1 Modeled SOC decomposition dynamics at an Ameriflux ponderosa pine forest in the United States (US-Me2). Subplot (a) – (d) are outputs from the dormancy model; (e), (g), (h) are outputs from the no-dormancy model. (f) is the measured soil temperature and volumetric moisture content at the site.
Figure 4.2 Modeled SOC decomposition dynamics at the larch plantation in northeastern China (CN-Lar). Note that this is a trenched plot. Subplot (a) – (d) are outputs from the dormancy model; (e), (g), (h) are outputs from the no-dormancy model. (f) is the measured soil temperature and volumetric moisture content at the site.
Figure 4.3 Parameters that are obtained after inverse modeling for dormancy model at all 6 sites. DB indicates deciduous broadleaf forest; EN indicates evergreen needleleaf forest.
difference between the two models (df=5, p<0.05). Thus, the magnitude of the oscillations in the dormancy model is significantly smaller than in the no-dormancy.

4.4.2 Inversed model parameters

Parameters that have biophysical meaning should reflect the patterns that characterize different ecosystem properties. Our mixed forest (CN-fixed) generally showed intermediate parameter values compared to deciduous broadleaf and evergreen needleleaf forests (Figure 4.3). Some parameters exhibited distinct patterns among deciduous broadleaf and evergreen needleleaf forests. For instance, microbial maintenance respiration (mR) was overall higher in evergreen needleleaf forests than deciduous broadleaf forests (Figure 4.3c), but the opposite was seen for initial active fraction (Figure 4.3l), indicating more stressed soil environment and higher energy limitation for microorganisms in evergreen needleleaf forests due to less substrate availability and poorer substrate quality. For other parameters, especially microbial and enzyme related parameters, the differences between the two major forest types were not significant (Figure 4.3f-i). Km is highest in US-MOz (Figure 4.3e), because it has the highest SOC content and the Michaelis-Menten formulation requires high Km to maintain the relative substrate level in a reasonable range. This also suggests the high sensitivity of the half-saturation constant to SOC in the Michaelis-Menten formulation.

4.4.3 Spatial extrapolations

4.4.3.1 Spatial distribution of soil $R_h$ and microbial biomass

The two models both simulated soil $R_h$ ranging between 300 and 1000 gC m\(^{-2}\) yr\(^{-1}\). The spatial pattern of the simulated soil $R_h$ of the dormancy and no-dormancy model
Figure 4.4 Simulated spatial pattern soil $R_H$ (a,b) and the MIC/SOC ratio (c,d) of the two models, where (a) and (c) are results from the dormancy model, and (b) and (d) are results from the no-dormancy model.
Table 4.4 Pearson correlation coefficient by grid cell between active proportion of microbial biomass (r) and soil properties, soil temperature and soil volumetric moisture for temperate forest.

<table>
<thead>
<tr>
<th>Soil physical and environmental factors</th>
<th>Dormancy Model</th>
<th>No-dormancy Model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>r (summer)</td>
<td>r (winter)</td>
</tr>
<tr>
<td>Bulk density (g cm(^{-3}))</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Particle density (g cm(^{-3}))</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Organic C content (mg cm(^{-2})) in the top 30 cm</td>
<td>0.03</td>
<td>0.04</td>
</tr>
<tr>
<td>Soil C:N ratio</td>
<td>-0.43***</td>
<td>-0.58***</td>
</tr>
<tr>
<td>Litterfall C input (gC m(^{-2}) yr(^{-1}))</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Annual mean soil temperature at 10cm</td>
<td>-0.19***</td>
<td>-0.28***</td>
</tr>
<tr>
<td>Annual mean soil volumetric moisture at 10cm</td>
<td>0.10***</td>
<td>0.12***</td>
</tr>
<tr>
<td>Soil volumetric moisture in summer</td>
<td>0.06*</td>
<td>0.07*</td>
</tr>
<tr>
<td>Soil volumetric moisture in winter</td>
<td>0.08</td>
<td>0.09**</td>
</tr>
<tr>
<td></td>
<td>(r) seasonal amplitude ((r_{\text{summer}} - r_{\text{winter}}))</td>
<td></td>
</tr>
<tr>
<td>Seasonal amplitude of soil temperature (summer - winter)</td>
<td>0.18***</td>
<td>0.03</td>
</tr>
<tr>
<td>Seasonal amplitude of soil volumetric moisture (summer - winter)</td>
<td>0.22***</td>
<td>-0.13**</td>
</tr>
</tbody>
</table>

* Significant at P<0.1; ** significant at P<0.05; ***significant at P<0.001
Figure 4.5 The spatial pattern of the active proportion of microbial biomass in summer and winter, and the C:N ratio of soil organic matter of the temperate forest latitudinal band (25°N-50°N).
differed in large areas of northwestern and southeastern US and in southern China, with the no-dormancy model simulating about 30% higher respiration than that of the dormancy model (Figure 4.4a,b). The soil $R_{H}$ of other regions was generally comparable between the two models. The total soil $R_{H}$ of all temperate forests from the dormancy model amounted to $7.28 \text{ PgC yr}^{-1}$, and $8.83 \text{ PgC yr}^{-1}$ for the no-dormancy model. While there may not be significant difference in the simulated spatial soil $R_{H}$ between the models, the MIC/SOC ratio showed distinct patterns in both magnitude and spatial distribution of the two models (Figure 4.4c,d). Here the MIC is the total microbial biomass including active and dormant microbes for dormancy model. The no-dormancy model overall simulated about two-times higher MIC/SOC ratio for temperate forests, especially in northern US, southern Europe, and northeastern China, than the dormancy model. In the no-dormancy model, the MIC/SOC ratio can reach about 4% (Figure 4.4d) whereas in the dormancy model the ratio ranged from 0.5% to 2% (Figure 4.4c). Grid cell based spatial correlation analysis showed that in both models, soil $R_{H}$ was negatively affected by bulk density and particle density (Table 4.4, $\rho \approx 0.25$, $p<0.001$), but had a significant correlation with soil C:N ratio ($\rho \approx 0.3$, $p<0.001$) and especially organic matter content ($\rho \approx 0.5$, $p<0.001$). In particular, our simulated spatial soil $R_{H}$ of temperate forests was high in the Great lakes regions in the US where SOC content was also reported high from the GSDE dataset (Figure 4.4a,b). Soil temperature and moisture also had significant positive effects on soil $R_{H}$ ($\rho \approx 0.3$ and -0.1, respectively, $p<0.001$), but were not as strong as the SOC.

4.4.3.2 Spatial pattern of microbial dormancy and its controlling factors
Annual active proportion of microbial biomass ranged from 2% to 20% across temperate forests (Figure 4.5a,b). The spatial distribution of active fraction was relatively the same across seasons. Seasonal active proportion of microbial biomass in summer was generally about 10% higher than in winter for large areas of northern US and northeastern China, whereas southern US, Europe and southern China featured relatively constant active fraction across seasons (Figure 4.5a,b). Grid cell based spatial correlation analysis showed that the soil C:N ratio was a major controlling factor on dormancy (Table 4.4, \( \rho = -0.43 \) in summer and \(-0.58\) in winter, respectively, \( p<0.001 \)), indicating higher nutrient availability (lower C:N ratio) is correlated with a lower dormancy proportion (higher active fraction). Annual temperature and moisture were weak controls on spatial dormancy pattern (\( \rho = 0.15 \)) except that winter active fraction had a slightly stronger negative correlation with annual temperature (\( \rho = -0.28 \), \( p<0.001 \)). However, temperature and moisture had very strong local controls on dormancy on temporal scales, with moisture had mostly strong positive temporal correlations with active fraction (\( \rho > 0.6 \), Figure 4.6a), as moisture was formulated to directly control substrate availability. Temperature showed negative temporal correlation with active fraction (\( \rho < -0.5 \), Figure 4.6b), primarily due to the negative covariation between temperature and moisture in the CCSM4 results (Figure 4.6c). It is worth noting here that, although annual temperature and moisture had weak controls on spatial patterns of active fraction, the seasonal amplitude of soil temperature and moisture generally exhibited higher correlations with that of active fraction (\( \rho > 0.18 \) and \( p<0.001 \), Table 4.4), suggesting high sensitivity of active-dormancy transition to seasonal changes in moisture and temperature levels on spatial scales.
**Figure 4.6** Temporal correlation (Pearson correlation coefficient) at each grid cell between (a) active proportion of microbial biomass and soil volumetric moisture content, (b) active proportion of microbial biomass and soil temperature, and (c) soil temperature and moisture content.
4.5 Discussion

4.5.1 Model performance and limitations

A synthesis by Bond-Lamberty et al. [2004] documented soil $R_H$ from temperate forests to range from 300 to 800 gC m$^{-2}$ yr$^{-1}$. We calculated the regional total soil $R_H$ based on reported mean value of 600 gC m$^{-2}$ yr$^{-1}$ and the land cover map used in this study and resulted in total soil $R_H$ to be around 7.11 PgC yr$^{-1}$. The dormancy model thus produced closer estimates to this synthetic estimate with 7.49 PgC yr$^{-1}$, whereas the no-dormancy model overestimated soil $R_H$ of 8.83 PgC yr$^{-1}$. Despite the comparable results between our simulated soil $R_H$ and synthesized observations, we used a simplified modeling framework without explicitly considering other key element cycles. Although we used soil C:N ratio to indicate substrate quality and its effects on microbial assimilation as a representative index, the coupled dynamics of kinetics and stoichiometric constrains on microbial physiology, which also pose key controls on decomposition dynamics, are not incorporated [Allison, 2005; Sinsabaugh et al., 2013; van Groenigen et al., 2006]. While the simplified framework may be sufficient to serve the purpose of this study, a more complex modeling scheme that accounts for the stoichiometry of other key elements should be able to reveal more biogeochemical controls which can then be benchmarked with observations to improve model performance.

4.5.2 Implications for informing experimental needs

Rainfall induced activation of dormant biomass can generate soil CO$_2$ pulses comparable in magnitude to the annual net C exchange of many terrestrial ecosystems, such as Mediterranean [Placella et al., 2012; Xu et al., 2004]. Particularly, such drying-rewetting events can exert stress on soil microbial communities and cause decrease in soil
basal respiration while total biomass increases [Fierer and Schimel, 2002]. In addition, changes in soil temperature and moisture conditions can induce responses in microbial basal respiration that were not explained by changes in total microbial biomass but rather changes in the physiology of soil microbial communities such as resuscitation of physiologically clustered microbial groups [Hagerty et al., 2014; Placella et al., 2012; Steinweg et al., 2012; Suseela et al., 2012]. In contrast to seasonal variation in soil R_H driven by changes in temperature and moisture in a variety of ecosystems [Suseela and Dukes, 2012; Suseela et al., 2012], total microbial biomass is generally unaffected by seasonality [Blume et al., 2002; Gunapala and Scow, 1998]. All of these indicate that soil respiration responses to environmental conditions are more closely associated with the active portion of microbial biomass than the total. Thus, the no-dormancy model that does not distinguish microbial biomass with different physiological states may not correctly represent the microbe-soil interactions. Similarly, using total biomass as an important metric in both experiments and modeling may also hinder effective data-model integration.

Our modeling results demonstrate that the ecosystem level controls (substrate quality and availability) on the average dormancy level (active proportion) at large spatial scales are different from those at local transient scales (temporal effects of soil moisture). This suggests that both site-level and spatial data should be used for model validation, because it is usually easier for model to reproduce site-level, short-term observations with data integration techniques, but much more difficult to capture spatial patterns [Todd-Brown et al., 2013] and long-term dynamics [He et al., 2014b]. In this study, we successfully reproduced soil R_H at six temperature forest sites, but our extrapolated soil
R_H revealed the potential issues with applying Michaelis-Menten kinetics on ecosystem scales and yielded high soil R_H in the northeastern US due to the high SOC content in that region. Such insufficiency in the model structure may not be disclosed at site-level examination. Therefore, spatially gridded comprehensive soil C and microbial physiology metrics would be tremendously helpful in model validation and assessment. For example, the contrasting controls of bulk density, particle density and organic C content on simulated soil R_H likely reflects covariation among these variables, because with increasing particle density C concentration decreased, implying that the soil organic matter accumulations were thinner [Sollins et al., 2009]. Our simulated soil R_H is then able to reflect the spatial controls of soil physical properties on decomposition.

Uncertainty in driving data for decomposition models may also be substantial and experimental measurements on large spatial scales would also be helpful. For example, the CCSM4 simulation we used cannot reproduce the surface frozen soil in northeastern China we observed in the site level measurements (Figure 4.2f), which potentially could introduce inaccuracies in model results. Note that in southern China broadleaf temperate forest does not show high temporal positive correlation of active proportion with soil moisture, this is likely because soil moisture is relatively constant throughout the year [Tang et al., 2006], thus soil moisture may not be the primary limiting factor on dormancy-active transitions in that region. More experimental data in that region should help benchmark both simulated soil moisture and temperature.

4.5.3 Implications for informing future model development

The high correlation between soil R_H and the organic C content in the top 30cm (Table 4.4) in our analysis may be attributable to the Michaelis-Menten kinetics we used
in the SOC enzymatic decay process (Eqn 4.1), where SOC content directly controls saturation level of the organic matter. Such high positive correlation between soil $R_{H}$ and the organic C content were not reported for other formulations (e.g., first-order kinetics in CMIP5 simulations where turnover time and net primary production are both positively correlated with SOC content across different earth system models) where decomposition rate is also associated with SOC content [Todd-Brown et al., 2013]. Thus we argue that Michaelis-Menten kinetics may not be suitable for characterizing the SOC enzymatic decay process when different soil layers are treated as one unified substrate. This is because the Michaelis-Menten kinetics have an implicit assumption that all substrate are accessible to enzymes under a homogeneous spatial distribution. The solution environment where Michaelis-Menten kinetics are usually applied is a good example that demonstrates the homogeneity requirement [Michaelis and Menten, 1913], thus Michaelis-Menten kinetics has a spatial constrain on relatively local scales. In addition, Michaelis-Menten formulation is derived under the assumption that enzymatic kinetics can cause a significant change on substrate levels [Michaelis and Menten, 1913], which is unrealistic for the microbial extracellular hydrolysis of SOC due to soil mineral-organic matter interaction and occlusion of SOC in soil aggregates which forms physical barriers [Ayati, 2012; Panikov and Sizova, 1996]. These limitations may explain the under-performance of the no-dormancy model at US-MOz site which has the highest SOC content among 6 sites. Although this issue is less notable in the dormancy model, its unrealistic spatial distribution of high soil $R_{H}$ in high SOC regions still suggests some issues of using Michaelis-Menten kinetics when treating a large SOC as homogeneous (Table 4.4). We propose that a better representation of soil vertical heterogeneity (e.g.,
would be essential to using Michaelis-Menten kinetics in microbial-based decomposition models. Large SOC content likely induced mismatch of the temporal scale of SOC change with that of microbial activity. To reconcile the homogeneity assumption of Michaelis-Menten dynamics and the localization of actual SOC enzymatic decay, vertical heterogeneity can be implemented using a multi-layer soil model structure or depth-resolved SOC profile thus ensuring certain degree of homogeneity of SOC and enzyme distribution at each depth increment [He et al., 2014b]. Stabilization of organic matter by interaction with poorly crystalline minerals is also a key mechanisms missing in current models [Ayati, 2012; Panikov and Sizova, 1996] and should be incorporated in future model development.

In both models, soil temperature and moisture exhibited similar levels of controls on soil RH (Table 4.4), this is likely attributed to the way soil moisture effect is defined in the model where it directly controls substrate availability. Such formulation with direct coupling with microbial activity can shed light on improving soil moisture representation in decomposition models as current first-order formulation in decomposition models only yield in marginal effects of soil moisture [Todd-Brown et al., 2013].

4.6 Conclusion

Microbial life-history traits such as dormancy play an important role in biogeochemical cycles. It has been widely observed that the active portion of microbial biomass, rather than the total biomass, explains the changes in microbial basal respiration rates. This study examines whether including dormancy in microbial-based soil decomposition model can improve the estimates of SOC dynamics and other microbial related metrics. Our results showed that although both dormancy and no-dormancy
models can capture the field observed soil $R_H$, the no-dormancy model exhibited larger seasonal oscillation and overestimation in microbial biomass. Our regional modeling results also indicated that models with dormancy were able to produce more realistic magnitude in microbial biomass and soil $R_H$, and that Michaelis-Menten kinetics may not be appropriate for models that do not vertically resolve decomposition dynamics in the soil profile. This study also identified the scale-dependent biogeochemical controls on microbial dynamics. Overall, our findings suggest future microbial model development should consider the representation of microbial dormancy, which will both improve the realism of microbial-based decomposition models and enhance the avenues for integration of empirical soil experiments and modeling.

4.7 Acknowledgement

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CHAPTER 5. CONCLUSION AND FUTURE WORK

This dissertation research highlights the importance of model-data integration in improving model predictability and constraining model uncertainties. This research also suggests that model intercomparison studies can be more efficient if a series of models share common features and their structures and parameters are compatible with measurements in terms of time step and modeled and observed variables. In this chapter, I first summarized answers to the research questions raised in Chapter 1. Second, I synthesized several recently published microbial models. Finally, I provided suggestions and directions for future microbial-based soil decomposition model development.

5.1 Summary for research questions

1) The model sensitivity analysis indicates that substrate availability (limited by soil water diffusion and substrate quality) is likely to be a major constraint on soil decomposition in the fibrous horizon, while energy limited microbial activity in the amorphous horizon exerts a predominant control on soil decomposition. Elevated temperature alleviated the energy constraint of microbial activity most notably in amorphous soils; whereas moisture only exhibited a marginal effect on dissolved substrate supply and microbial activity.

2) The model sensitivity analysis indicates that microbial related parameters have significant influence on modeled SOC dynamics, particularly, parameters that control
maximum microbial assimilation rate, enzymatic dynamics (turnover and production rate) and the Michaelis-Menten half-saturation constant. Thus, experimental work that can provide better constraints on these key parameters would be very helpful for model evaluation.

3) Both microbial-based and Q10 models with different soil layer architectures can reproduce the observed decomposition (heterotrophic respiration, \( R_H \)) from field studies reasonably well.

4) The long-term trajectories of soil C dynamics differ among traditional Q10 and microbial decomposition models. Specifically, Q10 models produced monotonic decreasing trend in SOC stocks under warming scenarios, whereas microbial model initially showed depletion of labile pools under warming and over time enhanced litterfall compensated the warming stimulated C loss, which aligns well with observations from long-term soil warming experiments.

5) The modeling analysis indicates that the dormancy model consistently produced a better match with field observed heterotrophic soil CO\(_2\) efflux (\( R_H \)) in comparison with the no-dormancy model. The regional modeling results further indicated that models with dormancy were able to produce more realistic magnitude in microbial biomass and soil \( R_H \). In contrast to strong temporal and local controls of soil temperature and moisture on microbial dormancy, soil carbon-to-nitrogen ratio (C:N) was a major regulating factor at regional scales, indicating scale-dependent biogeochemical controls on microbial dynamics.
5.2 Microbial model synthesis and future research directions

We surveyed 10 currently published microbial models that explicitly simulate microbial activities in SOC decomposition (Table 5.1). These models are all formulated with a set of ordinary differential equations, run at hourly time steps and fine spatial scales (cm$^3$), with state variables representing different C pools (thus the number of equations equals the number of state variables). Structurally, these microbial models usually consist of two or more pools of explicit SOC and separate pools for enzymes, microbial biomass, dissolved organic C, and sometimes a soluble C pool. The primary processes included are SOC enzymatic decay, microbial enzyme production and turnover of enzyme and microbial biomass. There is substantial overlap across models with respect to ecosystem processes (Table 5.2). However, mechanisms such as mineral adsorption/desorption, substrate/enzyme diffusion and microbial community dynamics and dormancy are less considered in these models. The majority of the models only consider C as a macronutrient, few models consider nitrogen.

Despite similar model structures, parameterizations and formulations are diverse across models. The representation of substrate and enzyme diffusion is either simplified as a function of volumetric soil moisture or uses empirical functions to account for solute diffusion rates (models 3,4). Microbial metabolic processes are primarily modeled as a maximum rate down-regulated by various modifiers that represent substrate and other physical conditions (model 1,2,3,4,5,6,8,9,10). Specifically, Michaelis-Menten kinetics is are commonly used to indicate substrate consumption (1,2,3,4,5,6,8,9,10), with various Q10 or Arrhenius-like functions being used to formulate the temperature dependence of
**Table 5.1** Structural and operational characteristics of 10 recently published microbial models.

<table>
<thead>
<tr>
<th>Model ID</th>
<th>Number of pools (number of ODEs)</th>
<th>Biogeochemical cycles simulated</th>
<th>Simulation spatial-temporal scales</th>
<th>Environmental dependencies included</th>
<th>Are soil processes vertically resolved?</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>C-only</td>
<td>hourly; cm$^3$ soil</td>
<td>Temperature</td>
<td>N</td>
<td>[Allison et al., 2010]</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>C-only</td>
<td>hourly; cm$^3$ soil</td>
<td>Temperature</td>
<td>N</td>
<td>[German et al., 2012]</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>C-only</td>
<td>hourly; cm$^3$ soil</td>
<td>Temperature, moisture</td>
<td>Y</td>
<td>[He et al., 2014]</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>C-only</td>
<td>hourly; m$^3$ soil</td>
<td>Temperature, moisture</td>
<td>N</td>
<td>[Manzoni et al., 2014]</td>
</tr>
<tr>
<td>5</td>
<td>10</td>
<td>C, N</td>
<td>Daily; mg soil</td>
<td>-</td>
<td>N</td>
<td>[Moorhead and Sinsabaugh, 2000]</td>
</tr>
<tr>
<td>6</td>
<td>9</td>
<td>C, N</td>
<td>daily; g soil</td>
<td>Temperature</td>
<td>N</td>
<td>[Schimel and Weintraub, 2003]</td>
</tr>
<tr>
<td>7</td>
<td>5</td>
<td>C-only</td>
<td>Hourly, daily and annual; whole soil column</td>
<td>Temperature</td>
<td>N</td>
<td>[Tang and Riley, in press]</td>
</tr>
<tr>
<td>8</td>
<td>10</td>
<td>C-only</td>
<td>hourly; mg soil</td>
<td>-</td>
<td>N</td>
<td>[Wang et al., 2014]</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>C-only</td>
<td>hourly; cm$^3$ soil</td>
<td>Temperature</td>
<td>N</td>
<td>[Wieder et al., 2014]</td>
</tr>
<tr>
<td>10</td>
<td>3</td>
<td>C, N</td>
<td>3 hour timestep, m$^3$ piece of litter</td>
<td>-</td>
<td>N</td>
<td>[Kaiser et al., 2014]</td>
</tr>
</tbody>
</table>
Table 5.2 Summary of common features of 10 recently published microbial models.

<table>
<thead>
<tr>
<th>Model features</th>
<th>Description</th>
<th>Environmental dependency/regulator</th>
<th>Model number</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pools</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOC (including litter)</td>
<td>Stable soil organic C substrates or polymeric organic C</td>
<td>-</td>
<td>1,2,3,4,5,6,7,9,10</td>
</tr>
<tr>
<td>SolubleC/DOC</td>
<td>Dissolved organic C or substrates that can be directly assimilated by microbes</td>
<td>-</td>
<td>1,3,4,5,6,7,8,10</td>
</tr>
<tr>
<td>MIC</td>
<td>Microbial biomass C</td>
<td>-</td>
<td>1,2,3,4,5,6,7,8,9,10</td>
</tr>
<tr>
<td>Ba/Bd</td>
<td>Active and dormant partitioned microbial biomass C</td>
<td>-</td>
<td>4,8</td>
</tr>
<tr>
<td>ENZ</td>
<td>Enzyme C</td>
<td>-</td>
<td>1,3,4,5,6,7,8,10</td>
</tr>
<tr>
<td>Reserved pool (part of MIC)</td>
<td>Internal metabolic buffer between microbial uptake and metabolism</td>
<td>-</td>
<td>7</td>
</tr>
<tr>
<td><strong>Fluxes/processes</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOC enzymatic degradation</td>
<td>Enzymatic decay of polymer SOC to monomers</td>
<td>Temperature, moisture</td>
<td>1,2,3,4,5,6,7,9,10</td>
</tr>
<tr>
<td>Fraction of DOC assimilated by microbes</td>
<td>Mineral adsorption may be involved; assimilation magnitude is calculated post hoc based on microbial respiration using constant CUE or prescribed function of CUE changing with temperature; dynamics energy budget theory based;</td>
<td>Temperature, DOC</td>
<td>1,3,4,5,6,7,8</td>
</tr>
<tr>
<td>Enzyme production</td>
<td>Enzyme production of microbes</td>
<td>Temperature, MIC</td>
<td>1,3,4,5,6,7,8,10</td>
</tr>
<tr>
<td>Microbial maintenance/growth respiration/metabolism</td>
<td>Microbial metabolic consumption to produce energy (CUE)</td>
<td>Temperature, MIC</td>
<td>4,5,6,7,8,10</td>
</tr>
<tr>
<td>Enzyme turnover rate</td>
<td>Rate of enzyme deactivation or loss; Mineral adsorption may be involved</td>
<td>Temperature, ENZ</td>
<td>1,3,4,5,6,7,8,10</td>
</tr>
<tr>
<td>Microbial turnover rate</td>
<td>Rate of microbial biomass turnover/death</td>
<td>MIC</td>
<td>1,2,3,4,5,6,7,8,9,10</td>
</tr>
<tr>
<td>Mineral surface adsorption/desorption of DOC and ENZ</td>
<td>Mineral surface binding of DOC and enzymes</td>
<td>Temperature</td>
<td>7,8</td>
</tr>
<tr>
<td>Diffusion of DOC and ENZ</td>
<td>Diffusion of DOC and ENZ in soil column</td>
<td>Temperature, moisture</td>
<td>3,4,7,8</td>
</tr>
<tr>
<td>Microbial functional groups</td>
<td>Explicitly represents different metabolic activity of microbial functional groups</td>
<td>-</td>
<td>9,10</td>
</tr>
<tr>
<td>Microbial community dynamics</td>
<td>Represents microbial communities made up of members with different life strategies</td>
<td>-</td>
<td>10</td>
</tr>
</tbody>
</table>
the maximum rate. A few models are based on thermodynamics or dynamic energy balance (Gibbs energy and entropy change) to quantify reaction rates (model 7).

Temperature sensitivity of soil carbon decomposition is modeled either as an emergent response (model 3,7), prescribed as constant Q10 (or Arrhenius activation energy) and/or carbon-use-efficiency (CUE)/growth yield (model 4,5,6,8), or an empirical function (e.g., linear) of temperature (1,2,9). Soil moisture effects on decomposition through controlling substrate transport are only represented in a few models (3,4) and most models focus only on temperature effects. Enzyme production and deactivation rate and microbial death rate are commonly modeled either as a fixed or temperature-dependent proportion of microbial biomass or as an absolute rate change in mass. Only two models (model 5,6) explicitly considered the effects of nutrient (nitrogen) on microbial and SOC dynamics.

Based on the above synthesis of recent models and the studies included in this dissertation, there are several suggestions for future microbial-based modeling and field research.

For model developers,

1) Given the mechanistically-based framework of the microbial models, the biophysical meaning of most parameters, and the reported parameter sensitivity analysis, closer collaboration between model development and experimental tests is recommended. Specifically, modeled microbial functional response should be benchmarked with measured environmental perturbations. The model parameters should be designed in a
way so that they can be constrained by experimental data directly.

2) Our overview for existing models highlights that there are a number of directions to explore the importance of incorporating new details to microbial models, including: a) heterogeneity in space and time caused by properties of the external environment such as soils, drainage conditions and vegetation; b) model representation of a diversity of microbial life-history traits and microbial community dynamics; and c) model representation of multiple macro and micro limiting nutrients.

For experimentalists,

1) Given the common structure in recently published microbial models, some key microbial physiology metrics should be measured along with other specific variables of interest. While many experiments have examined the response of microbial respiration to temperature in laboratory microcosms, very few includes multiple measurements of microbial function that drives models, such as microbial and enzyme turnover, and carbon use efficiency (CUE), which are commonly seen across different models.
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VITA
VITA

Yujie He received a Bachelor of Science with a major in Environmental Science from Fudan University, Shanghai, China, in May 2010. In August 2010, she entered the Graduate School of Purdue University and enrolled in a Ph.D. program in Ecological Science and Engineering, with Department of Earth, Atmospheric and Planetary Sciences as her home department. During the following 4 years, she obtained a Master of Science with a major in Atmospheric Science in 2012 and continued to finish her doctoral degree in December 2014.
PUBLICATIONS


Submitted/In progress