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Boreal soil carbon dynamics under a changing climate: A model inversion approach

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[1] Several fundamental but important factors controlling the feedback of boreal organic carbon (OC) to climate change were examined using a mechanistic model of soil OC dynamics, including the combined effects of temperature and moisture on the decomposition of OC and the factors controlling carbon quality and decomposition with depth. To estimate decomposition rates and evaluate their variations with depth, the model was inverted using a global optimization algorithm. Three sites with different drainage conditions that represent a broad diversity of boreal black spruce ecosystems were modeled. The comparison among the models with different depth patterns of decomposition rates (i.e., constant, linear, and exponential decrease) revealed that the model with constant inherent decomposition rates through the soil profile was able to fit the observed data in the most efficient way. There were also lower turnover times in the wettest site compared to the drier site even after accounting for moisture and temperature differences. Taken together, these results indicate that decomposition (especially for the wetter site) was not accurately represented with standard moisture and temperature controls and that other important protection mechanisms (e.g., limitation of O_2, redox conditions, and permafrost) rather than low inherent decomposition rates are responsible fer the recalcitrance of deep OC. The simulation results also showed that most of the soil CO_2 efflux is generated from subsurface layers of OC because of the large OC stocks and optimal moisture conditions, suggesting that these deeper soil OC stocks are likely to be critically important to the future carbon dynamics.

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1. Introduction

[2J The global mean temperature increased approximately 0.74°C in the past 100 years mainly due to the emissions of anthropogenic greenhouse gas (e.g., CO_2 and CH_4) from various sources (e.g., agricultural and industry) and will further increase 1.1-6.4°C during the 21st century *[intergovernmental Panel 011 Climate Change,* 2007]. This warming trend is expected to be more pronounced in the boreal region *[Gihhard et al.,* 2005], which contains approximately 30-60%) of the world's terrestrial soil OC *[Gorham, 1991; Hohhie et al.,* 2000; *Lal,* 2005]. This high latitude region has been the subject of significant research effort in recent years due to the large carbon reservoirs, which might play an important role in the feedback between the global carbon cycle and climate change *[Dunn et al.,* 2007]. The increasing temperature can, in principle, stimulate the decomposition rate of OC *[Serreze et al.,* 2000; *Wickland and Neff,* 2007], reduce the thickness and duration of snow cover *[Beniston,* 1997], degrade permafrost *[Osterkamp and Romanovsky,* 1999; *Sazonova et al.,* 2004; *Zhang et al..* 2005], and increase the frequenoy of wildfire *[Flannigan et al.,* 2005; *Gillett et al.,* 2004]. All these effects collectively may increase the CO_2 flux from the soil OC to atmosphere, and result in a positive feedback to the warming atmosphere. However, the OC losses due to these positive feedbacks could be partially or completely offset by the increases in OC stocks caused by increasing productivity or changes in the soil physical regime that could include both wetting and drying trends. Both precipitation and evapotranspiration patterns, as well as the corresponding water movement in the vadose zone, are expected to change with the warming climate in the boreal region *[Gurdak et al., 2007; Soja et al.,* 2007] but with uncertain implications for soil carbon dynamics.

[3] The decomposition of OC depends on the complex interactions between moisture content and temperature and is inhibited at both low and high moisture content *[Wickland and Neff,* 2007]. As a result, changes in moisture dynamics (if soils become very dry or very wet) may be a critical control on future carbon dynamics in boreal soils. These potential trajectories of change represent the considerable uncertainty that surrounds the fate of boreal OC under a changing climate.

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[4] A number of computer simulation models have been developed to study the role of various important factors in the future boreal and global soil OC dynamics. These factors include wildfire [*Balshi et al.,* 2007; *Harden et al., 2000; Randerson et al.,* 2006; *Rupp et al.,* 2007], soil thermal dynamics [*Euskirchen et al.,* 2006; *Thornley and Cannell,* 2001; *Zhuang et al.,* 2003; *Zhuang et al., 2001],* soil drainage condition [*Manies et al.,* 2003], land use and vegetation changes [*Calefet al.,* 2005; *Marland et al., 2003; McGuire et al.,* 2001], permafrost [*Dutra et al., 2006; Lawrence and Slater,* 2005], dissolved organic carbon (DOC) [*Neff and Asner,* 2001], nutrient availability [*Rastetter et al.,* 2004], snow cover [*Euskirchen et al.,* 2006; *Stieglitz et al.,* 2003], and growing seasons [*Euskirchen et al., 2006; Frolking et al.,* 1996]. Despite these many modeling approaches, there remains considerable uncertainty regarding boreal OC responses to climate change [*Davidson and Janssens,* 2006]. One ofthe basic uncertainties in boreal OC cycle predictions comes from the unusual nature of these soils in comparison to temperate settings and limited understanding of the full suite of environmental controls on OC release in boreal settings. For example, the response of OC to the increasing soil temperature has been given significant consideration in the existing models, while comparatively little attention has been paid to other important environmental factors (e.g., moisture or oxygen content). The structure of boreal soils compounds these issues because of relatively deep (>0.5 m), OC rich layers of soil, that are difficult to simulate with conventional models that focus on surface soil OC dynamics.

[5] Temperate soil OC is typically assumed to have increasing recalcitrance of OC with depth as well as increased physical protection of OC stocks [*Baisden et aI.,* 2002; *Davidson and Janssens,* 2006]. In boreal soils, the change in inherent recalcitrance (e.g., fundamental chemical properties that protect OC from decomposition) ofOC with depth is still not clear due to the limited data and little to no physical stabilization of carbon onto mineral surfaces or into aggregates. However, boreal soils often contain permafrost andlor cold and saturated subsurface soil layers that may act to preserve carbon over long time scales. These differences with temperate systems suggest that boreal soils may operate in a fundamentally different manner. Moreover, many studies have suggested that that the deep OC pool might have a positive feedback to climate change [*Rapalee et al.,* 1998; *Trumbore and Harden, 1997].* Taken together, it is necessary .to better understand the importance of deep OC in the boreal soil OC budget [*Dioumaeva et al.,* 2003; *Trumbore and Harden, 1997].*

[6] In addition to questions regarding the structure and function of boreal soils, there are also uncertainties in model predictions that arise hom the structure of conceptual models (e.g., overparameterization or deficiencies) [*Son and Sivapalan,* 2007], parameter identification, data availability and quality, initial and boundary conditions, and errors associated with numerical implementation. Most of the simulations of current ecosystem and carbon models were designed in a factorial combination of predefined factors or parameters, also known as direct problems. The major difficulty associated with the direct problems is that the reliability of simulations on carbon dynamics is highly dependent on the quality of the predefined parameters (e.g., decomposition rates of various OC fractions). In many cases, some parameters arc difficult or impossible to obtain from laboratory measurements. For example, it is impossible to use current available techniques to separate fine, coarse, and humic OC from the boreal OC pools and then measure thc rates of decomposition (or turnover time) for each OC fraction. As a result, the low quality of the predefined decomposition rates used in the carbon models could likely result in the low reliability of model simulations,

[7] The objective of the study was to improve our understanding of the sensitivity of boreal soils (especially the deep OC) to elimate warming by incorporating the variations of decomposition rates with depth into an existing soil OC dynamics model. The improved OC dynamics model was then tested on three different sites (a dry site without permafrost, a dry site with permafrost, and a poorly drained site with permafrost) that largely represent the complexity and uniqueness of boreal soils. A model inversion approach (also known as parameter optimization) was used to reliably estimate the important parameters associated with the OC decomposition for the three sites. Wc then used the estimated parameters to study the vulnerability of boreal soil OM under a changing climate.

2. Methods

2.1. Site Descriptions

[8] Three black spruce forest sites with different soil drainage type, OC layer thickness, and bulk OC density were simulated in thc study, and fully described in Table 1.

2.2. Model Descriptions

[9] The soil OC dynamics model used in this study was based on a multiple pool boreal soil OC model developed by *Carrasco et al.* [2006]. Since the model structure has been well described in the original paper, only a brief description will be presented here. In the model, the soil OC pools were divided into three tractions: fine (e.g., moss and fine root), coarse (e.g., coarse root), and humic OC. The dynamics of soil OC layers through time were captured by developing a new regrowing surface OC layer following each fire event, while older OC accumulates to form a multiple layer soil structure. The total OC layers, therefore, will be equivalent to the number of fire events plus the regrowing surface layer. Another novel aspect of this OC model is the ability to simultaneously evaluate the distribution of carbon isotopes (i.e., ^{13}C and ^{14}C)through layers (or depth) over time. This constraint on model dynamics allows an additional mechanism by which to evaluate the goodness of model simulations by comparing thc modeled and observed carbon isotope profiles. The simulations by *Carrasco et al.* [2006] were defined as a direct problem and designed in a factorial combination of several factors (e.g., NPP, fire severity, and fire return interval, etc) with fixed decomposition rates for fine, coarse, and humic OC. In this study, the simulations were defined as an inversion problem and approached by inversely estimating the paramcters (OC decomposition rates and their depth patterns) that were not available in the literature and difficult or impossible to obtain by laboratory measurements. The following will present only the improvements and modifications

Table 1. Descriptions of the Three Black Spruce Forest Sites

Site Name	DFTC	DFCC	NOBS
Sampling time	2000	2001	1994
Location[a]	Tower control site within the Donnelly Flats region, located at 63°53.322′N and 145°44.439′W near Delta Junction, Alaska.	Creek control site within the Donnelly Flats, located at 63°50.932′N and 145°42.777′W, near Delta Junction, Alaska.	Northern study area Old Black Spruce site of the boreal ecosystem and atmosphere study, located at 53°59.1′N and 105°7.32′W, near Thompson, Manitoba, Canada.
Slope	<5°	<5°	<5°
Drainage type	Well drained (dry site)	Well drained (dry site)	Poorly drained (wet site)
Permafrost	Without permafrost	With permafrost	With permafrost
Total mass of OC above the mineral soil[a]	2.93 kg OC m^{-2}	3.16 kg OC m^{-2}	23.8 kg OC m^{-2}
Soil profile[a,b,c]	0–2 cm: live moss, lichen, and litter; 2–4 cm: dead moss and litter; 4–5 cm: slightly decomposed OC and roots; 5–10 cm: moderately decomposed OC; 10–11 cm: moderately decomposed OC with charcoal; below 11 cm: mineral soil	0–1 cm: live moss, lichen, and litter; 1–3 cm: dead moss and litter; 3–14 cm: amorphous material; 14–15 cm: moderately decomposed OC; 15–19 cm: well decomposed OC with charcoal; below 19 cm: mineral soil	0–4 cm: live moss; 4–30 cm: dead moss; 30–41 cm: dead moss and dead roots; 41–64 cm: humified organic matter; below 64 cm: mineral soil

[a]From *Manies et al.* [2004].
[b]The soil horizons were classified on the basis of the method proposed by *Harden et al.* [2006].
[c]The site description for NOBS is from *Carrasco et al.* [2006] and *Sellers et al.* [1995].

(temperature and moisture regulation; depth regulation; layer thickness calculation), which were made to the Carrasco model to better investigate the OC decomposition rates and distributions in the soil. For other important parameters, assumptions, and processes, please refer to the original paper *[Carrasco et al., 2006]*.

2.2.1. Temperature and Moisture Regulations

[10] The variable sensitivity of soil OC decomposition to temperature in temperate and forest soils has been discussed in a number of studies *[Davidson and Janssens,* 2006; *Lis/a et al.,* 1999; *Thornley and Cannell,* 2001]. Recently, a series of incubation studies on the decomposition of boreal soil OC under various moisture and temperature conditions were conducted by *Wickland and Neff* [2007]. The results (Figure 1) indicated that moisture content had a strong effect on decomposition at various temperatures, while the effect of temperature on decomposition was significant between 50 and 75% saturation (water filled pore space divided by

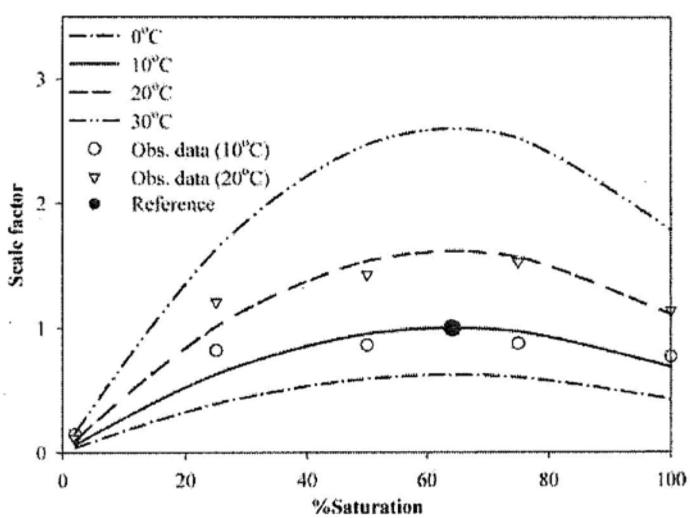

Figure 1. The decomposition rates determined on the basis of the work of *Wickland and Neff* [2007] using equation (1). The parameters a, b, and θ_c in equation (1) were estimated on the basi of the observed data at 10 and 20°C. The fitted results were $a = 1.514$, $\theta_c = 0.642$, and $b = 0.048$. The curves for 0 and 30°C were calculated using equation (1) with the estimated parameters a, b, and θ_c. Note that the decomposition rates were shown as scale factors $[K(\theta, T, x)/k^*]$, where $K(\theta, T, x)$ is the actual decomposition rate and k^* is the reference inherent decomposition rate at $\theta = \theta_c$ (i.e., 0.642) and $T =$ 10°C.

the total pore space) and was negligibly small at the low percent saturation. To describe the combined effects of temperature and moisture on decomposition, a mathematical equation was developed on the basis of the work of *Wickland and Ncdl*[2007] and defined as

$$K'(\theta, T) = k* \times \left[\left(\theta_c^2 - (\theta - \theta_c)^2\right) \times ae^{bT}\right], \quad (1)$$

where (-) *is* the percent saturation, *T* is the soil temperature (^{o}C), (-) is the optimal percent saturation corresponding to the maximum K^{-1}((-), T), and $k*$ is the reference inherent decomposition rate (the ideal decomposition rate without any environmental controls) at (-) = $(-)_c$ and T = 10°c. The actual decomposition rate, K^1((0), T),.will be adjusted up and down on the basis of equation (1). For a constant (-), the K^1(!J, T) exponentially changes with T on the basis of the relationship ae^{bT} (a Q_{10} response). There are three unknown parameters in equation (-), $(-)_c$, *a*, and *b*, which were estimated by fitting equation (1) to the observed decomposition rates at 10^{o}C and 20^{o}C with various percent saturation (Figure 1). The fitted results were $a = 1.514$, $(-)_c$ = 0.642, and $b = 0.048$. Note that this relationship was only available when temperature was above 0 ^{oC}. *Dioumaeva et al.* [2003] and *Michaelson and Ping* [2003] reported that some decomposition was observed for feather moss peat when soil temperature was below 0°C due to the presence of large amounts of liquid water, especially for the interval of ~2°C to 0.08°C. Therefore, it was assumed in our model that the decomposition rates between - 2 and 0^{o}C were 30% of the values calculated at 0^{o}C with the same percent saturation on the basis of the results of *Dioumaeva et al.* [2003], and no decomposition occurred below -2°C.

2.2.2. Depth Regulation

[II] In the previous model, *Carrasco et al.* [2006] and many other oe models, such as Century *[Parton et al., 1987; Parton et al.,* 1988] and Rothe *[Coleman et al.,* 1997], the decomposition rates for different oe fractions (fine, coarse, and humic) are assumed to be an inherent property of carbon. In other words, after removal of environmental controls on decomposition, different pools will still have different turnover times as the result of inherent physical or chemical properties (e.g., different oe structure). In most soil organic matter models, vertical soil profiles are not simulated and when depth is addressed [e.g., *Carrasco et al.*, 2006], the lack of data on turnover times with depth forces an assumption that decomposition rates are invariant from surface to deep soil oe pools. By contrast, many studies have reported that the deep old organic OC was usually more recalcitrant (resistant to decomposition) than the top young organic OC for the same oe fraction (for example, the top young and deep old fine oe might have different turnover time). *[Fontaine and Barot,* 2005; *Fontaine et al.,* 2007; *Schoning and Kogel-Knabner,* 2006; *Sollins et al.,* 1996; *Trumbore, 2000].* Despite the apparent increases in turnover times and hurnification with depth, it is currently very difficult to make assumptions about how decomposition rates change with depth in soils. There are many factors causing thc recalcitrance of deep OC. These factors include lower inherent decomposition rates and differing mixes of more labile (readily decomposable) to more recalcitrant pools. More discussions on these factors will be provided later. To use a model inversion approach to evaluate possible change in decomposition rates with depth, wc hypothesized that the inherent decomposition rates were a function of depth and defined as

$$K(\theta, T, x) = K'(\theta, T) \times \left(1 - cx^d\right)$$
$$\begin{cases} c = 0 & \text{for constant } K \text{ with depth(Model 1)} \\ c \neq 0, \text{and } d = 1 & \text{for linear decrease in } K \text{ with depth (Model 2)} \\ c \neq 0, \text{and } d < 1 & \text{for exponential decrease (concave up)in } K \text{ with depth(Model 3)} \\ c \neq 0, \text{and } d > 1 & \text{for exponential decrease(concave down)in K with depth (Model 4)} \end{cases} \quad (2)$$

where *x* is the OC layer depth (cm), c is the "substrate factor" in which larger values indicate more recalcitrance, and *d* is an "attenuation exponent" by which recalcitrance of substrate *c* declines. If $c = 0$, then we surmise that there is no difference in inherent decomposition rate, or substrate recalcitrance. c and *d* are the unknown parameters that were estimated in the model inversion depending on the type of model.

2.2.3. Layer Thickness Calculations

[12] The thickness of each OC layer was determined on the basis of the mass and bulk density of fine, coarse, and humic oe at that layer, and was defined as

$$Z_{OC} = \sum_{j=1}^{m} Z_j = \sum_{j=1}^{m}\left(\frac{{}^F\text{Mass}_j}{{}^FBD_j} + \frac{{}^C\text{Mass}_j}{{}^CBD_j} + \frac{{}^H\text{Mass}_j}{{}^HBD_j}\right), \quad (3)$$

where *m* is the number of OC layers, *BD* is the bulk density (g cm-^{3}) Zj is the thickness of OC layer, j (cm), Zoc is the total thickness of OC layers (cm), and superscripts *F*, *C*, and *H* represent fine, coarse, and humic OC. The bulk OC densities of fine, coarse, and humic OC for the three sites were 0.014, 0.029, and 0.54 g oc cm^{-3}. respectively. These bulk OC densities were the average values of samples taken at various locations and depths across the three black spruce forest regions *[Manies et al.,* 2003; *Trumborc et al.,* 1998]. This approach to calculate layer thickness is significantly different from the use of an empirical relationship between the accumulated oe mass and depth by *Carrasco et al.* [2006], which might lead to inaccurate calculation of layer thickness (for example, 1 kg of fine OC and 1 kg of humic OC might give the same layer thickness by *Carrasco et al.* [2006]). Note that mineral fractions of oe layer was eliminated from equation (3) because mineral fractions contributed less than 5% of the thickness of OC layer due to the small mass and high bulk density compared to OC pools.

2.3. Input Data Sets

2.3.1. Temperature, Moisture, and Radiocarbon Profile Distributions

[13] Radiocarbon profile distributions for DFTC and DFCC were obtained from *Manies et al.* [2004]. Monthly average soil temperature and moisture content for DFTC was measured using thermocouples (Model 105T, Campbell Scientific) and Time Domain Reflectorneters (Model CS615. Campbell Scientific) *[Winston et al.,* 1997]. Data for DFCC was measured using negative temperature coefficient thermistors (Model No. 14A5001C2, Alpha Sensors, Inc.) and Stevens- Vitel Hydra probes (Stevens Water Monitoring System. Inc.) *[Manies et al.,* 2003]. The thermistors were calibrated at USGS laboratory facilities and the accuracy of these thermistors was ±0.0 1°C. The Hydra probe outputs were converted from millivolts to moisture content using correction values from K. Yoshikawa (personal communication, University of Alaska at Fairbanks, 2003). DFTC data were recorded at depths of 2, 4, 11, and 37 cm for soil temperature and moisture content. DFCC data were recorded at depths of 2, 4, 15, 25, and 40 cm for moisture content, and 2, 5, 9, 15, 25, and 70 cm for soil temperature. For NOBS, soil temperature and moisture content were recorded at depths of 7.5, 22.5, 45, 75, and 105 cm *[Carrasco et al.,* 2006J.

2.3.2. Fire Return Interval and Severity

[14] For NOBS. the tire return interval was 200 years and the last historical fire year was 1880 *[Carrasco et al.,* 2006J. The fire return intervals were 80 and 150 years with the last historical fire years for DFTC and DFCC at 1921 AD and 1886 AD, respectively *[Mack et al.,* 2007; *Manies et al.,* 2003]. A fire severity of 20% of available fuels was assumed in the model following the simulation by *Carrasco et al.* [2006J and *Hardenet al. [2000].*

2.3.3. Net Primary Productivity

[15] The total net primary productivity (NPP) was separated into three fractions: stem, branch, and foliage NPP; moss NPP; and root NPP. The root NPP was further separated into coarse root NPP (15%) and fine root NPP (85%) *[Carrasco et al.,* 2006]. In the model simulations, the total fine OC input was equivalent to the sum of moss NPP and fine root NPP, while the total coarse OC input consists of coarse root NPP and standing dead inputs that fall and enter the soil as stems and branches. For DFTC and DFCC, the aboveground NPP was 0.134 kg OC m^{-2} a^{-1} (where a is years; consisting of 0.018 kg OC m^{-2} a^{-1} of moss and 0.116 kg OC m^{-2} a^{-1} of stem and branch) and 0.125 kg OC m^{-2} a^{-1} (consistin▌ of 0.025 kg OC m^{-2} a^{-1} of moss and 0.1 kg OC m^{-2} a^{-1} of stem and branch) *[Mack et al.,* 2007J, respectively. The belowground NPP (i.e., root NPP) was derived on the basis of the empirical relationship reported by *Steele et al.* [1997] and *Ruess et al.* [2003], who reported that the root NPP contributed approximately 40- 60%, of total NPP for black spruce forests in Saskatchewan and Manitoba, Canada. On the basis of their result, the root NPP for DFTC and DFCC in the model simulations was set equal to the aboveground NPP. As a result, the total NPP for DFTC and DFCC was 0.268 kg OC m^{-2} a^{-1} and 0.25 kg OC m^{-2} a^{-1}. For NOBS, the stem and branch NPP, moss NPP, and root NPP was 0.05, 0.074, and 0.1 kg OC m^{-2} a^{-1}, respectively, following the simulation for this site by *Carrasco et al. [2006].*

[16] The root input zones for DFTC, DFCC, and NOBS were set to 0-11 cm, 0-19 cm, and 20-50 cm, respectively *[Carrasco et al.,* 2006], indicated as depth from the moss surface as it accumulates. Root biomass distribution in the root zone has a significant effect on the radiocarbon profile distribution. The coarse root biomass in the model was evenly distributed through the entire root zone on the basis of the field observation, while the fine root biomass followed an exponential probability density distribution (PDF) *[Carrasco et al.,* 2006; *Steele et al.,* 1997] that is defined as

$$\mathrm{PDF} = \mu e^{-\mu(x - x_{root})} \tag{4}$$

and the corresponding cumulative distribution function (CDF) is defined as

$$\mathrm{CDF} = 1 - e^{-\mu(x - x_{root})}, \tag{5}$$

where x is the OC layer depth (em), x_{root} is the depth of root zone surface (em), and p is the rate parameter. Note that the coarse and fine root biomass was set to zero when $x - x_{root}$ was greater than the thickness of root zone. There is one unknown parameter u in the equations (4) and (5). Additional constraints must be applied to uniquely estimate the parameter u. *Steele et al.* [1997] reported that approximately 70% of fine root of black spruce in the Canadian boreal region was found in the upper half of the root zone. Therefore, to determine the parameter u., the following constraints were set to equation (5),

$$\begin{aligned} &\mathrm{CDF} \to 0.7 \quad \text{at the half of root zone} \\ &\mathrm{CDF} \to 1.0 \quad \text{at the bottom of root zone.} \end{aligned} \tag{6}$$

The estimated rate parameter *(u)* for DFTC, DFCC, and NOBS was 0.229, 0.138, and 0.087.

2.4. Parameter Estimation

[17] The inversion problem in this study was to seek the minimization of the objective function (also called cost function). Obj. which was defined as

$$\mathrm{Obj} = W_c \times \left(\mathrm{TOC} - \overline{\mathrm{TOC}}\right)^2 + W_d \times \left(Z_{OC} - \overline{Z_{OC}}\right)^2 + \sum_{i=1}^{n} W_i \left({}^{14}C_i - \overline{{}^{14}C_i}\right)^2, \tag{7}$$

subject to

$$\begin{cases} 0.007(\mathrm{a}^{-1}) \le k^*_{\mathrm{fine}} \le 12(\mathrm{a}^{-1}) \\ 0.007(\mathrm{a}^{-1}) \le k^*_{\mathrm{coarse}} \le 12(\mathrm{a}^{-1}) \\ 0.007(\mathrm{a}^{-1}) \le k^*_{\mathrm{humic}} \le 12(\mathrm{a}^{-1}) \\ 10^{-6} < c < 1.0 \quad \text{for Model 1, 2, and 3}, \\ 0.05 < d < 1.0 \quad \text{for Model 3} \\ 1.0 < d < 10.0 \quad \text{for Model 4} \\ k^*_{\mathrm{humic}} \le k^*_{\mathrm{coarse}} \le k^*_{\mathrm{fine}} \end{cases} \tag{8}$$

where TOC is the amount of total OC mass (kg OC m^{-2}); Zoc is the total thickness of OC layer (cm); $^{14}C_i$ is the measured ^{14}C at depth of i (%,); n is the number of data points; $\overline{\mathrm{TOC}}$, $\overline{Zoc}$, and $\overline{^{14}C_i}$ are the predicted values using the model with a given set of parameters; W_c, W_d, and W_i are

Table 2. Results of Parameter Estimates for DFTC, DFCC, and NOBS With Different Models Using Equations (1) and (2)

	Model 1	Model 2	Model 3	Model 4	Observed Value
		DFTC			
k^*_{fine} (a^{-1})[a]	0.682	0.718	0.714	0.716	–
k^*_{coarse} (a^{-1})	0.577	0.585	0.645	0.644	–
k^*_{humic} (a^{-1})	0.514	0.521	0.526	0.518	–
c	0.0	0.006	0.022	0.008	–
d	–	1.0	0.502	1.078	–
C layer thickness (cm)	11.039	11.038	11.019	11.016	11.000
Heterotrophic CO_2 efflux (kg m^{-2} a^{-1})	0.251	0.252	0.252	0.252	–
Total SOC (kg m^{-2})	2.623	2.643	2.611	2.627	2.93
		DFCC			
k^*_{fine} (a^{-1})	0.896	0.900	0.942	0.883	–
k^*_{coarse} (a^{-1})	0.567	0.579	0.594	0.578	–
k^*_{humic} (a^{-1})	0.316	0.348	0.336	0.345	–
c	0.0	0.002	0.028	0.0007	–
d	–	1.0	0.260	1.206	–
C layer thickness (cm)	19.125	19.018	19.053	19.039	19.000
Heterotrophic CO_2 efflux (kg m^{-2} a^{-1})	0.231	0.231	0.231	0.235	–
Total SOC (kg m^{-2})	5.123	5.020	5.123	5.008	3.160
		NOBS			
k^*_{fine} (a^{-1})	0.077	0.078	0.081	0.074	–
k^*_{coarse} (a^{-1})	0.071	0.073	0.075	0.073	–
k^*_{humic} (a^{-1})	0.037	0.037	0.037	0.041	–
c	0.0	0.0005	0.024	0.0001	–
d	–	1.0	0.147	1.200	–
C layer thickness (cm)	68.442	69.413	68.947	69.435	64.000
Heterotrophic CO_2 efflux (kg m^{-2} a^{-1})	0.232	0.234	0.235	0.232	–
Total SOC (kg m^{-2})	18.363	18.811	18.914	18.023	23.800

[a]Here k^* represents the reference inherent decomposition rate at θ = 0.642 and T = 10°C (see equation (1)).

the weighing function. W" Wl, and ~ were set to 1000, 1000, and 1, respectively, resulting in a lower weight on *Zoe* and approximately equal weight on TOC and 6.^{14}C in the objective function. In equation (7), the first term represents the relative deviation (RO) in total OC mass, the second term represents the RO in total OC thickness, and the third term represents the sum of squared error (SSE) for the radiocarbon profile. There are three (for Model I), four (for Model 2), or five (Model 3 and 4) parameters to be estimated, kt,ne, "-'tmuse, ktumic, *c* (as a substrate factor) and! or *d* (as an attenuation exponent by which the recalcitrance of substrate factor *c* declines). The upper and low bounds (equation (8)) for the estimated parameters were defined on the basis of the following two rules: the bounds (1) should have physical meanings and (2) be large enough to contain all possible solutions.

[18] Because of the nature of nonlinearity, models like the OC dynamics model in this study are known to be frequently ill posed and have many local optima *[Banga et al.,* 2003]. The traditional local optimizations (e.g., gradient based) are not suitable to find the best or unique solutions. A global optimization, stochastic ranking evolutionary strategy (SRES) *[Runarsson and Yau,* 2000, 2005], was used to inversely estimate the parameters. SRES has been demonstrated by many studies to be the most robust and eftieient global optimization strategy *[Banga et al., 2003; Moles et al.,* 2003]. libSRES (version 1.0) *[Ji and Xu,* 2006], coupled with an ordinary differential equation solver, CVODE (version 2.5.0) *[Cohen and Hindmarsh,* 1994], was used to solve the SRES problem. Because of the expensive computation, a portable implementation of the message passing interface, MPICH2 (version 1.0.6pl) *[Gropp et al.,* 2007], was used for parallel computation to reduce the computational efforts.

[19] In the model, the sensitivity and uncertainties of estimated parameters could not be evaluated using either bootstrap resampling or Markov Chain Monte Carlo simulation because of the huge computational efforts and complicated theoretical derivation. To overcome these difficulties is still a great challenge for long time scale ecosystem modeling. The development of efficient algorithms and improvement of available computational resources might provide us a means to address these difficulties and limitations in the future,

2.5. Simulations of Future Carbon Dynamics

[20] To further explore the response of OC to warming for sites with different drainage, long-term future projections on OC storage and CO_2 efflux were also evaluated for the three different study sites using the best fit parameters hom the above inversion exercises. Four different warming scenarios (O°C, 2°C, 5°C, and 10°C) were simulated for the period 2000-2600 to examine the potential response of OC dynamics to climate change. The conditions at year 2000 were used as the initial conditions for the simulation. It should be noted that the OC dynamics at year 2000 were at nonequilibrium condition (net OC loss) because of the assumption of 2°C warming during the period 1500-2000 in the OC model *[Carrasco et al.,* 2006]. The temperature was assumed to linearly increase during the prediction period to the designated temperature. The moisture profile, depth patterns of decomposition rates, NPP, and other factors except temperature were held constant.

3. Results

[21] The results of the model inversion for optimal conditions ((-) = 0.642 and T = 10°C) (Table 2 and Figure 2) indicated that DFTC and DFCC have the similar inherent decomposition rates (i.e., k^*_{fine}, k^*_{coarse}, k^*_{humic} in Table 2) ranging from 0.942 a-1 (1.1 years of turnover time) for tine OC to 0.316 a- 1 (3.2 years of turnover time) for humic oc. Compared to DFTC and DFCC, the decomposition rates {or NOBS were very low and ranged from 0.081 a-1 (12 years of turnover time) for fine OC to 0.037 a^{1} (27 years of turnover time) for humic OC.

[22] Overall, the observed radiocarbon profiles (Figure 2) were well matched with the estimated profiles for DFTC and OFCC, while the radiocarbon profile for NOBS was partially mismatched in all four models, especially for the two data points (at the depths of 19 and 23 cm) located at the interface between the top young OC layer and root zone (ranged from 20 to 50 cm). The results also indicated that the differences between estimated total OC mass and OC thickness among the four models for DFTC, DFCC, and NOBS were small. The differences in estimated radiocarbon profile distributions among the four models were evaluated using a two-sample t-tcst (heteroscedastic, two-tail distribu-

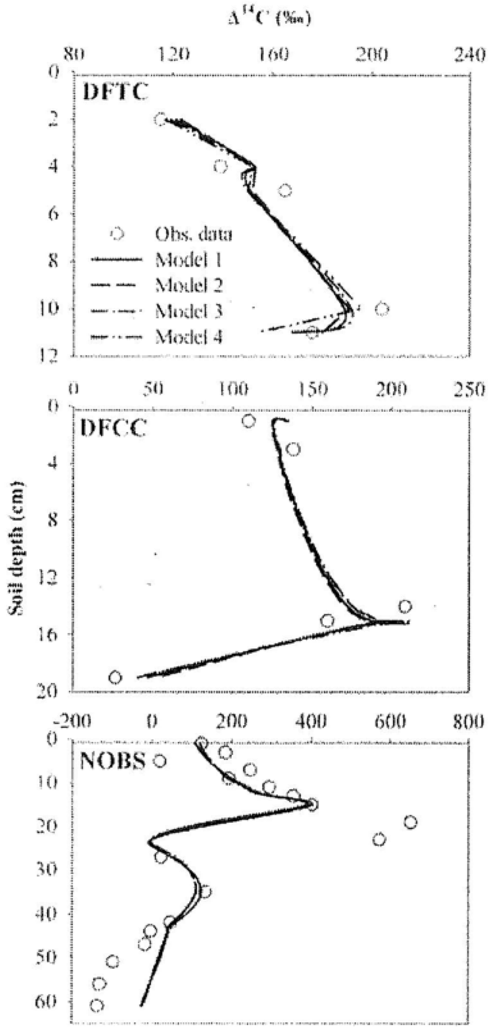

Figure 2. The observed and estimated radiocarbon profiles at year 2000, 2001, and 1994 for DFTC, DFCC, and NOBS, respectively. Model 1, 2, 3, and 4 are defined in equation (2).

tion). The test results indicated that the t values ranged from 0.098 to 0.164 for DFTC, from 0.011 to 0.058 for DFCC, and from 0.01 to 0.035 for NOBS. These t values are less than the critical values (2.306 for both DFTC and DFCC, and 2.032 for NOBS), suggesting that differences in ^14C profiles among the four models were not significant (although model 3 was slightly better than other three models). Moreover, the inherent decomposition rates calculated from Models 2, 3, and 4 decreased approximately 8-11% for OFTC, 2-6% for DFCC, and 2-4% for NOBS from the top OC to the deep OC. Taken together, the model with constant inherent decomposition rates through the soil profile (Model 1) was the simplest (least number of free parameters) yet good enough to represent the depth patterns of inherent decomposition rates in the OC profile.

[23] The distributions of actual decomposition rates through the soil profile for each month for DFTC, DFCC, and NOBS were calculated using equations (l) and (2) with Model 1 and presented in Figure 3 with decomposition rates provided as scale factors. The inherent decomposition rate k^* at (-) = 0.642 and $T = 10^{o}$C (defined in equation (1)) was defined as 1. The actual decomposition rates at different times of the year and different depths were determined by multiplying the corresponding scale factors found in Figure 3 with the decomposition rates listed in Table 2 (for Model I). The results illustrate that the depth patterns of actual decomposition rates for DFTC and DFCC were more similar to the moisture profiles than temperature profiles, while for NOBS (wet site) actual decomposition rates were better matched with the temperature profiles, especially for the high decomposition rates.

[24] The results of future projections on OC storage and heterotrophic CO_2 efflux are shown in Figure 4. Notc that the peaks in Figure 4 represent the wildfire events. The predictions indicate that warming will lead to significant reductions of soil OC (56-78%) and CO_2 efflux (5-25%) in the future for the poorly drained site, but such reductions are small for the two dry sites (8-40% and 8-20% reductions in soil OC for OFTC and OFCC, respectively, and relatively constant CO_2 efflux) because of the insensitivity of decomposition to temperature at low moisture content (Figure 4). The future simulations with O°C warming also indicate that the poorly drained site has a longer equilibration time, exceeding 300 years, in response to temperature perturbations during 1500-2000 than the dry sites (~100 years).

4. Discussion

[25] One of the great challenges of model inversion is to seek the best set of parameters that can reproduce the observations and measurements [*Moles et al.*, 2003]. Global optimization approaches allow the use of global information to analyze the interactions between parameters and search for the global optimum [*Stephens and Baritompa*, 1998], in contrast to the local optimization that only uses local information (e.g., derivative values) resulting in high sensitivity to the initial values of the estimated parameters and producing only local minima. The global optimization approach (i.e., SRES), along with the strictly defined multi-criteria objective function, in this study provided the reliable means to use easily measured data (i.e., ^14C profile and total OC mass and thickness) to estimate parameters that are difficult to obtain or measure directly, and therefore provide more mechanistic insight into the OC dynamics.

4.1. Landscape Level Variation in Decomposition Rates

[26] The inversely estimated decomposition rates using field observations with our model were similar to those obtained from laboratory incubation studies by *Wickland and Neff* [2007], who reported that the average turnover time of near-surface OC ranged from 3.1 to 5.4 years for OFTC and OFCC at the same temperature and similar moisture content. Our results also indicated that the turnover times for NOBS were slower than those for DFTC/DFCC. The differences of decomposition rates between DFTC/DFCC and NOBS might be partially due to several factors including differences in substrate quality or decomposer community or due to environmental factors that were not

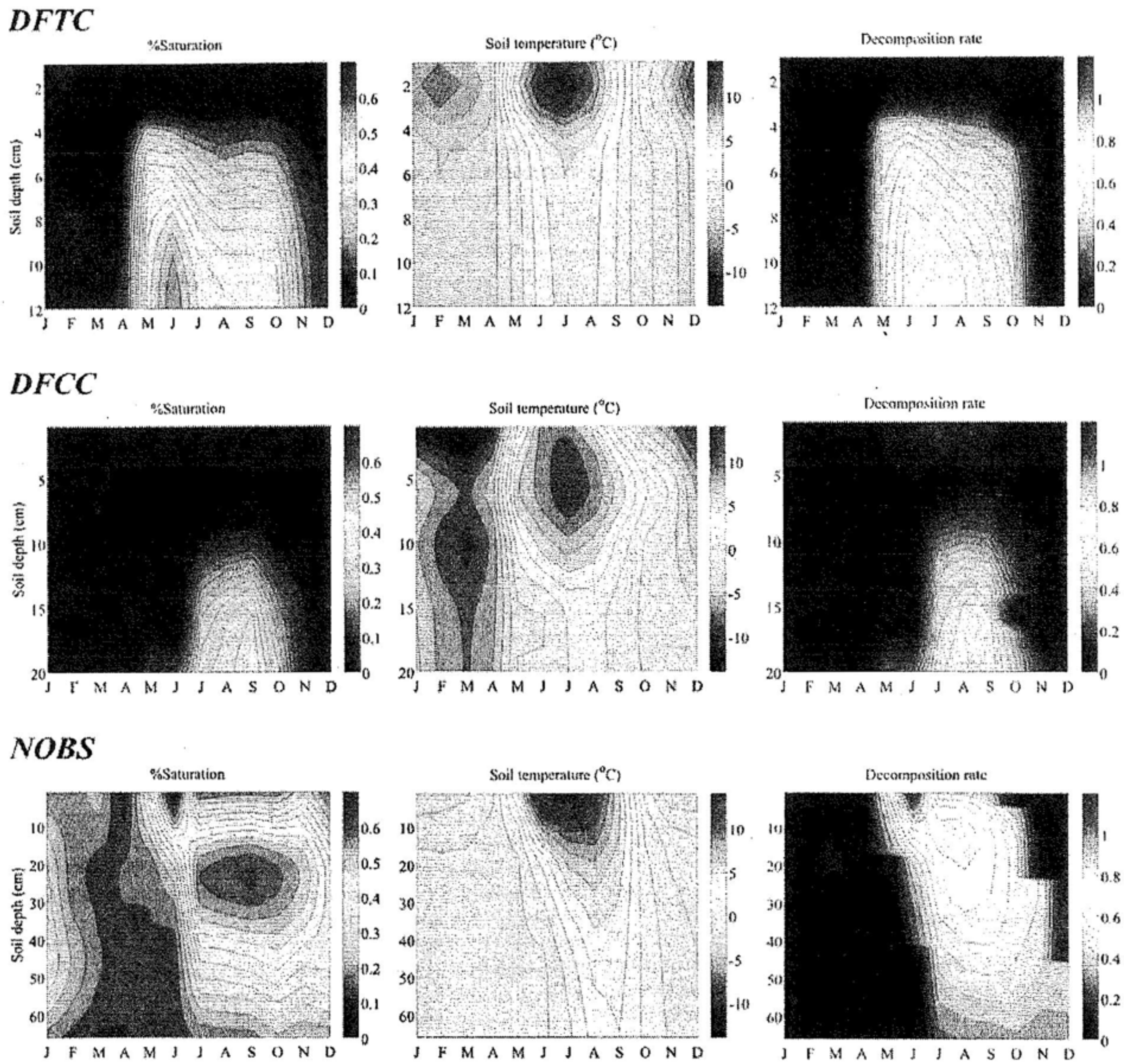

Figure 3. Monthly average temperature, percent saturation, and actual decomposition rates calculated using equations (1) and (2) with Model 1. The actual decomposition rates were expressed as scale factors $[K(\theta, T, x)/k^*]$, where $K(\theta, T, x)$ is the actual decomposition rate and k^* is the reference inherent decomposition rate at $\theta = 0.642$ and $T = 10°C$. Note that the decomposition rate profiles for DFTC and DFCC were similar to the percent saturation profiles, while the decomposition rate profile for NOBS was similar to the temperature profile.

considered in this modeling exercise. There is evidence that moss species differences can affect vegetation decomposition because of the production of antimicrobial agents, the lack of lignin structures, and/or different decomposition pathways [*Dioumaeva et al.,* 2003; *Turetsky,* 2004], however these effects are not typically of the magnitude suggested by this study.

[27] The results of this study indicate dramatically slower decomposition rates for NOBS compared to the drier sites. It is possible that SOM structural differences are responsible for differences in decomposition potential hut most studies of dry and wet sites in boreal and arctic setting suggest that when soils are incubated under common conditions (despite differences in field drainage conditions), the soil OC tends to decompose similarly and relatively quickly [*Neff and Hooper,* 2002; *Wickland and Neff;* 2007]. Although it is possible that soil structure and/or differences in the microbial community structure are responsible for the apparent wet/dry contrast in inherent k values, these factors alone seem insufficient to account for the relatively large differences.

[28] The environmental conditions ill wet and dry sites in boreal settings are strikingly different. These differences include variations in temperature, moisture conditions and the seasonality of both environmental factors. To a large

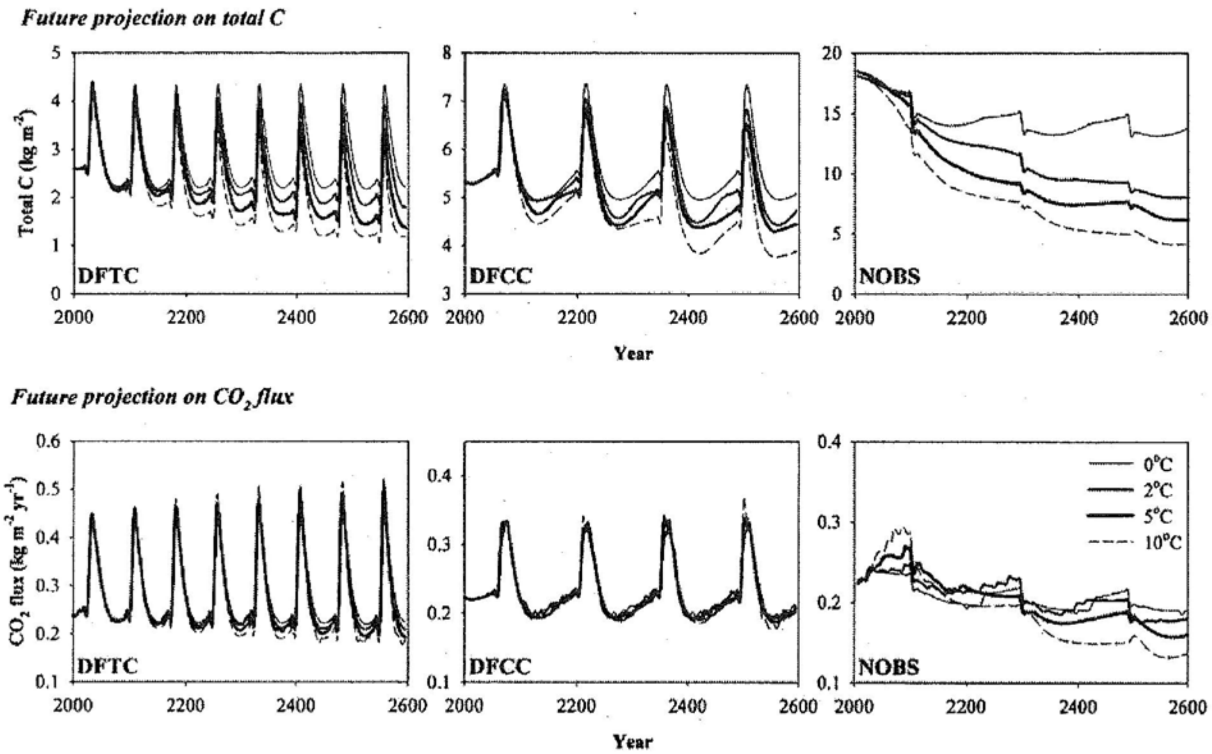

Figure 4. Future projections on total OC mass and heterotrophic CO_2 efflux with various warming scenario (0, 2, 5, and 10°C) for the period 2000–2600. The future projections were simulated using the estimated parameters for Model I (Table 2). The peaks represent the wildfire events. Note the nonequilibrium condition (net OC loss) at year 2000 due to the 2°C warming for the period 1500–2000 assumed in the model [*Carrasco et al.*, 2006].

degree, the direct effects of these factors should be accounted for in our inversion exercise through the temperature and moisture scalars used in the inversion. There are additional indirect effects, sueb as oxygen availability and DOC, which are influenced by soil physical properties (e.g., moisture) but are not fully incorporated into this model for reasons discussed below.

[29] Oxygen availability is a key component of anaerobic decomposition but it is also a process that is currently difficult to model for boreal settings for several reasons. Oxygen availability in soils is controlled by a complex mixture of factors that include moisture content, biological activity and soil structural characteristics that influence gas diffusion. One notable aspect of moisture in the three sites is that the high moisture content in DFTC and DFCC sites was observed at the bottom of OC soil layers, but in the middle of OC layers (approximately 20-30 cm) in NOBS. In this wet site, the middle zone of OC layers with high moisture content could become a barrier to block the gas diffusion from the surface to the deeper soils. Further, considering the oxygen consumption in the root zone below this barrier (ranging from 20 to 50 cm), it is not unreasonable to assume that subsurface soil OC pools would periodically undergo anaerobic decomposition because of the limitation of O_2 in NOBS. In the anaerobic conditions, NO^{-3}, Mn+4, $Fe^{+3,}$ and $S0_2^{-4}$(instead of $O_{2)}$ in order serve as the electron acceptors [*Korom,* 1992]. The high activation energies associated with these electron acceptor reactions would slow the rates of deep and old OC decomposition. Because we do not currently represent these factors in the model, these environmental controls would appear as lower "inherent" decomposition rates for NOBS compared to the drier sites.

[30] Second, one other factor may influence the wetter sites and that is the presence of historical permafrost that may have slowed decomposition in the relatively recent (~100 years) past. Both the DFCC and NOBS likely had shallower active layers in the recent past [*Beltrami et al.,* *1995; Osterkamp and Romanovsky, 1*999]. The presence of historical permafrost at the NOBS site was inferred by *Carrasco et a1.* [2006] modeling exercises and may also be a factor in the slow inherent *k* that resulted from the inversion. The overall results ofthis study suggest that there is a striking difference between the potential decomposition of dry and wet sites in boreal settings and although the exact causes of these differences are currently difficult to identify, the potential importance of drainage conditions on soil OC stability is clear.

[~1] Finally, the stable carbon isotope signatures would be transferred from topsoil to subsoil in the form of DOC resulting in the redistribution of ^{14}C in the soil profile, which might be responsible for the mismatch between the observed and estimated radiocarbon profile for NOBS. The decomposition of the deep and old OC might also be stimulated and enhanced by DOC which would carry fresh

OC and/or labile OC providing the energy for microorganisms or enzyme to maintain biological activities and to breakdown the recalcitrant OC *[Fontaine and Barot, 2005; Fontaine et al.,* 2007; *Vance and Chapin,* 2001). Although some models [e.g., *Neff and Asner,* 2001] were developed to explore the role of DOC in terrestrial ecosystems, it is still a challenge to incorporate the fate and transport of DOC within soil OC models. Simulation of DOC fluxes are complicated by interactions with other environmental controls due to simultaneous fate and transport processes (e.g., advection, dispersion, decomposition, attachment and detachment of DOC, and transformation among OC fractions), complex physical properties of media (e.g., transient water flow and variable hydraulic conductivity associated with the variable moisture content), and very complex hydrologic flowpaths in boreal settings. Because information on those important parameters and hydrologic pathways is still quite limited, additional experiments and data are necessary to model the transport of DOC across boreal landscapes.

[32] The discrepancies between the observed and estimated radiocarbon profile for NOBS might be partially due to the missing of important environmental factors (c.g., oxygcn availability, permafrost, and DOC transport) in our model which have been fully discussed earlier. Also, on the poorly drained site (especially peatland), aboveground litter input (i.e., moss and foliate) would be accumulated each year to form a multilitter-cohort-layered structure, and 14C signature in each litter cohort is independent *[Frolking et al.,* 2001; *Hanson et al.,* 2005]. A single regrowing surface layer used in our model might not be able to capture such cohort-based ^{14}C signatures, leading to a mismatch between the observed and estimated ^{14}C profile for NOBS. These results collectively highlight the importance of developing models of boreal soils that are capable of simulation the unique environmental conditions of these settings.

4.2. Soil Organic Matter Structure

[33] One of the basic questions in modeling soil carbon dynamics is what representation of soil pools is most appropriate *[Kirschbaum,* 2000; *Yu et al.,* 2001a, 2001b). In the temperate zone, there is good evidence that a multiple pool structure is critical for soil carbon modeling *[Baisden et al.,* 2002; *DeGryze et al.,* 2004; *Heim and Schmidt, 2007; Knorr et al.,* 2005]. In this study, the influence of pool structure on model performance varied by site. The inherent decomposition rates among the three OC pools for DFTC were not very different (i.e., a single OC pool captured most ofthe variation in parameterization). In DFCC and the NOBS site, the inherent decomposition rates of humic OC were approximately two to three times slower than those of tine and coarse OC, These long turnover times result in the long equilibration time tor OC in the future climate simulation.

[34] There are at least two explanations for the differences in among OC pools; they are as follows:

[35] 1. The shallow OC layer (~cm) in DFTC allows the fine roots (providing fresh and/or labile OC) to reach the deep humic OC pools and promote the decomposition rates of humic OC as discussed earlier. This is supported by high root counts in the humic layers of DFTC (Field Descriptions *[Manies et al.,* 2004]). By contrast, DFCC has very few roots in the humic layer. Therefore, the inherent decomposition rates of humic OC for DFTC would be overestimated if the positive impact of fine roots on the inherent decomposition rates of humic OC was missing in equations (1) and (2).

[36] 2. The slowing of the turnover in the humic layers of the DFCC site, which experiences periodic saturation of soils, may also represent moisture-oxygen interactions in deeper soil layers.

4.3. Soil Organic Matter Structural Distribution

[37] The simulation of the distributions of various OC fractions through the profile at the end of the model run for all three sites (Figure 5) indicates that tine and coarse OC dominate the OC pools at thc surface layers while humic OC dominates the deep OC layers. Note that the hulk density of humic OC is approximately foul' times greater than those affine and coarse OC, resulting in large OC mass stocks in the deep OC layers. This simulation (Figure 5) also indicated that the heterotrophic CO_2 efflux from the deep OC layers was approximately two to twelve times greater than from the top OC layers, owing mainly to higher moisture content in the lower layers. These results are consistent with large contrasts between *kS/l<l/1".,.* and *k",.<'l'* tor a variety of soil drainage types in the Manitoba study environments *[Trumbore and Harden,* 1997]. These results further suggest that the subsurface OC stocks play an important role in contemporary fluxes of CO_2 from soil decomposition due to the optimal moisture conditions and large OC storage in these layers. This simulation is similar to the results of incubation studies by *Dioumaeva et al.* [2003], who reported that humic OC pool contributed 30-50% (annually) of respiration sources in feather moss and sphagnum peats. Given this important current role in OC exchange, it is reasonable to expect that these layers will also playa dominant role in the response of boreal systems to climate change as suggested by a number of investigations *[Blodau et al.,* 2007; *Czimczik et al.,2006; Trumbore and Harden,* 1997; *Turetsky et al., 2007].*

[38] In this simulation, we used one Q_{10} value for all the soil fractions but there is emerging evidence that OC derived from different vegetation types (e.g., feather moss versus Sphagnum moss) may have different Q_{10} values suggesting an interaction between OC structure and temperature responses *[Dioumaeva et al.,* 2003; *Wickland and Neff;* 2007]. *Knorr et al.* [2005] suggested that thc non labile OC pool has a higher Q_{10} value (more sensitive to temperature) than labile OC pool. This result together with the simulation results discussed earlier (i.e., large humic OC pool and optimal temperature and moisture) indicates that the potential vulnerability of deep OC might be exacerbated if individual Q_{10} values were applied to each OC fraction.

5. Conclusions

[39] The results of inverse modeling indicate that the old subsurface OC and the young shallow OC generally have the similar inherent decomposition rates for each OC fraction (i.e., fine, coarse, and humic). The deep humic layers form mainly by a process of slow burial, particularly during postfire reaccurnulation *[Harden et al.,* 2000], but this study suggests that preservation of the deep layers is largely controlled by environmental conditions rather than inherent structural differences in these fraction. Similarities in the inherent (not actual) decomposition rates for shallow

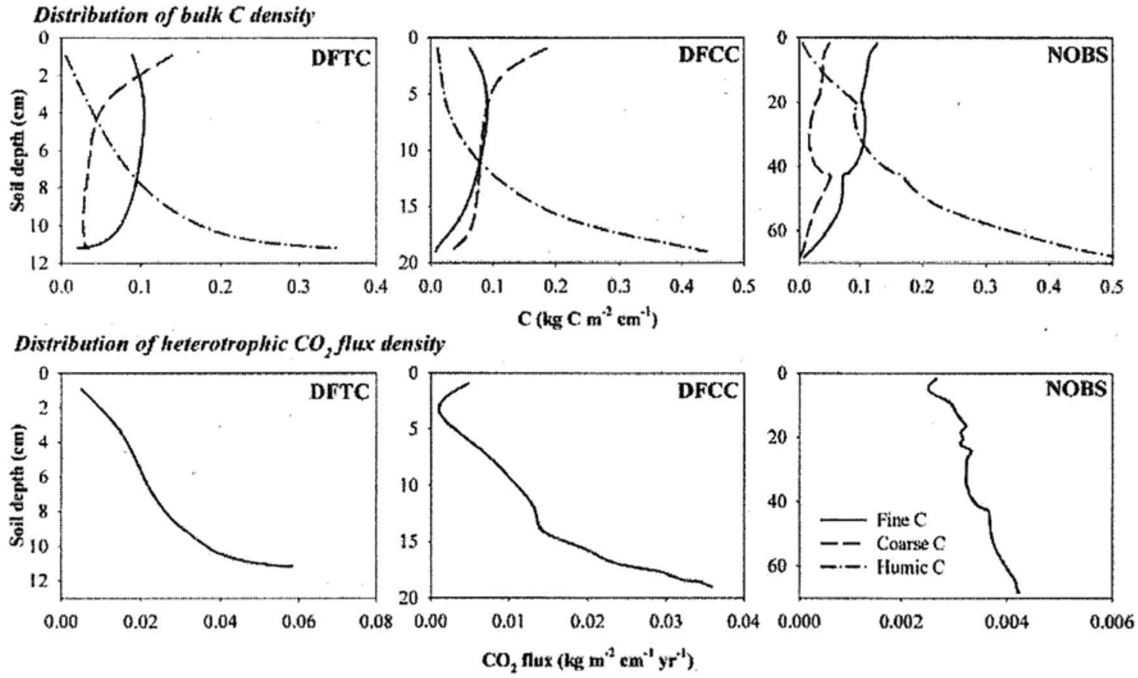

Figure 5. The simulated (top) bulk OC density and (bottom) heterotrophic CO_2 efflux density distribution through the depth for the three OC fractions (fine, coarse, and humic) at year 2000 for DFTC, DFCC, and NOBS. Please note that the large OC stocks at the deep soil profile due to the high bulk OC density.

and deep substrates suggests that inherent decomposition rates obtained from the surface OC can be applied to the subsurface OC as well. Across soil moisture gradients, however, there appears to be either less homogeneity in the inherent *k* of organic matter or a suite of additional environmental and/or biological controls that act to provide additional protection of carbon in wetter soil settings. As boreal landscapes continue to change into the future, the role of soil drainage and changing hydrologic conditions is likely to become of paramount importance. Much attention has been paid to the role that temperature will play in control of future carbon exchange between boreal ecosysterns and the atmosphere [*Davidson and Janssens,* 2006; *Dioumaeva et al.,* 2003; *Liski et al.,* 1999; *Thornley and Cannell,* 2001], however this study and recent field studies [*Wickland and Neff;* 2007] suggest that moisture could potentially bc more important to the fate of the large stocks of boreal carbon in a changing climate.

[40] An important assumption in our model is that the N PP and moisture content profiles arc constant during the simulations including future projections. Increasing temperature would extend the growing season and result in greater NPP [*Bond-Lamberty et al.,* 2004]. This inerease would at least partially offset· the loss of C from the soil due to the temperature increase. Also, the soil moisture and thermal dynamics depend on permafrost dynamics, topographic conditions, and soil thawing-freezing processes as well as precipitation and snow cover [*Euskirchen et al., 2006).* Finally, losses of OC as CH_4 to the atmosphere or as DOC to the groundwater, which are not included in our model, are also important factors to the OC dynamics in the boreal soils. These important issues will be addressed in the future modeling work when our current model is incorporated into other existing ecosystem models. Nonetheless, the current simulations provide a starting point for a revised prediction of how boreal soils may respond to climate change.

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