



Equifinality in parameterization of process-based biogeochemistry models: A significant uncertainty source to the estimation of regional carbon dynamics

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[1] Numerical biogeochemistry models suffer from equifinality problem in their parameterizations using eddy flux tower data, which can contribute to diverged estimates of regional carbon dynamics. To date, the uncertainty in regional estimates propagated from the site-level parameterization equifinality has not been well characterized. Here, we use a process-based biogeochemistry model, the Terrestrial Ecosystem Model (TEM), and a Bayesian inference framework to quantify the influence of parameterization equifinality on the estimates of carbon dynamics in boreal forest ecosystems during the 20th century. By conducting three groups of ensemble regional simulations, we find that, given a certain climate data set being used, (1) in comparison to the effects of random noises in climate forcing, the regional uncertainty due to parameterization equifinality is remarkably greater, (2) the parameterization equifinality results in drastically different decadal variations in the estimation of carbon storage during the 20th century, and (3) the uncertainties associated with parameterization equifinality and random noises in climate forcing vary both spatially and seasonally. We conclude that the equifinality from site-level parameterizations in biogeochemistry models is an important uncertainty source in estimating regional carbon dynamics. Simply extrapolating the site-level parameterization to large spatial and temporal scales could bias the regional estimates irrespective of regional climate data sets used in our analysis. Ensemble process-based biogeochemistry model simulations conditioned on observed ecosystem fluxes with Bayesian inference techniques could provide more serious estimates of regional carbon dynamics and their associated uncertainties.

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1. Introduction

[2] Earth system models usually have multiple interactive physical, chemical, and biological components and are mathematically formulated with numerous equations and parameters associated with their processes and controls [Entekhabi and Eagleson, 1989; Beven and Binley, 1992]. Equifinality in parameterizations of these models has long been recognized to affect the model predictability and uncertainty [e.g., Beven and Binley, 1992; Beven, 1996; Franks *et al.*, 1997; Beven and Freer, 2001; Schulz *et al.*, 2001]. Parameterization equifinality occurs when different sets of parameters for a single modeling system result in same or similar predictions, given that the model, forcing data and observations used in calibration are not perfect

[Beven and Freer, 2001]. For example, in a previous study, we have demonstrated that a biogeochemistry model, the Terrestrial Ecosystem Model (TEM), when calibrated against eddy flux tower data, is able to reproduce the observed carbon (C) fluxes with similar accuracy, but with very different sets of parameters (J. Tang and Q. Zhuang, A global sensitivity and Bayesian inference framework to improve the parameter estimation and prediction of process-based terrestrial ecosystem models, submitted to *Global Change Biology*, 2008, hereinafter referred to as Tang and Zhuang, 2008), for a black spruce ecosystem in Canada. Thus, given the same model structure, climate forcing, and initial conditions, there is not a unique set of parameters, which could be used for regional extrapolation. Rather, Bayesian theory suggests that all the parameters derived with Bayesian inference technique have a certain probability to be a “true” set of parameters [Tarantola, 2005]. If we simply extrapolate one set of those possibly “true” parameters to a region with biogeochemistry models, the regional estimates of carbon dynamics will potentially be seriously biased.

[3] In the past, in quantifying the uncertainty of regional estimates of carbon dynamics due to site-level parameterization equifinality, biogeochemistry models have been

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Table 1. TEM Parameter Values for the Base Simulations at Black Spruce Forest Ecosystem in Bonanza Creek, Alaska, and the Standard Simulations in the Northern Study Area of BOREAS, Manitoba, Canada^a

Name	Unit	Definition	Base Simulation	Standard Simulation	Prior Range
k_c	$\mu\text{L/L}$	Half saturation constant for $\text{CO}_2\text{-C}$ uptake by plants	100	195.72	[20, 600]
k_i	$\text{J cm}^{-2} \text{d}^{-1}$	Half saturation constant for PAR use by plants	75	50.353	[20, 600]
T_{\min}	$^{\circ}\text{C}$	Minimum temperature for GPP	-8.0	-5.4756	[-12, -4]
T_{optmin}	$^{\circ}\text{C}$	Minimum optimum temperature for GPP	5.5	5.8262	[0, 15]
T_{optmax}	$^{\circ}\text{C}$	Maximum optimum temperature for GPP	20.0	19.037	[15, 25]
T_{\max}	$^{\circ}\text{C}$	Maximum temperature for GPP	29.0	31.191	[25, 35]
RAQ10A0	None	Leading coefficient of the Q10 model for plant respiration	2.35665	2.7679	[1.3502, 3.3633]
RAQ10A1	$^{\circ}\text{C}^{-1}$	First-order coefficient of the Q10 model for plant respiration	-0.053077	-0.051222	[-0.054577, -0.051183]
RAQ10A2	$^{\circ}\text{C}^{-2}$	Second-order coefficient of the Q10 model for plant respiration	0.0023842	0.0023061	$[2.2902, 2.4381] \times 10^{-3}$
RAQ10A3	$^{\circ}\text{C}^{-3}$	Third-order coefficient of the Q10 model for plant respiration	-4.110×10^{-5}	-3.9835×10^{-5}	$[-4.17, -3.97] \times 10^{-5}$
k_{n1}	g/m^3	Half saturation constant for N uptake by vegetation	4.2	4.8716	[0.5, 10]
k_{n2}	g/m^3	Half saturation constant for N uptake by heterotrophic organisms	4.2	3.8209	[0.5, 10]
MINLEAF	None	Minimum photosynthetic capacity of vegetation	0.5	0.50327	[0.2, 0.8]
ALEAF	None	Coefficient to model the relative photosynthetic capacity of vegetation	0.42893	0.28868	[0.1, 1.0]
BLEAF	None	Coefficient to model the relative photosynthetic capacity of vegetation	0.33295	0.11575	[0.1, 1.0]
CLEAF	None	Coefficient to model the relative photosynthetic capacity of vegetation	0.32228	0.41158	[0.0, 0.5]
MOISTOPT	% saturation	Optimum soil moisture content for R_H	0.5	0.54753	[0.2, 0.8]
RHQ10	None	Change in R_H rate due to 10°C temperature increase	2.00	2.4991	[1, 3]
CMAX	$\text{g m}^{-2} \text{mo}^{-1}$	Maximum rate of photosynthesis C	768.07	1656.75	[216.65, 1666.65]
CFALL	$\text{g g}^{-1} \text{mo}^{-1}$	Proportion of vegetation carbon loss as litterfall monthly	0.0020.37	0.00048062	[0.0001, 0.015]
KRC	None	Logarithm of plant respiration rate at 0°C	-6.467	-4.7447	[-7.5, -3.5]
KDC	$\text{g g}^{-1} \text{mo}^{-1}$	Logarithm of heterotrophic respiration rate at 0°C	0.00216527	0.005868	[0.000906, 0.007406]
NMAX	$\text{g m}^{-2} \text{mo}^{-1}$	Maximum rate of N uptake by vegetation	374.6775	397.8875	[171.8375, 871.8375]
NFALL	$\text{g g}^{-1} \text{mo}^{-1}$	Proportion of vegetation nitrogen loss as litterfall monthly	0.007955	0.0054617	[0.003, 0.012]
NUP	g/g	Ratio between N immobilized and C respired by heterotrophs	29.2639	48.5549	[9.9019, 104.9019]
VEGC2N	g/g	Mean C:N of vegetation	375.0	462.45	[200, 600]

^aThe prior ranges are based on the studies of *Raich et al.* [1991] and *McGuire et al.* [1992], except for T_{\min} , T_{optmin} , T_{optmax} , T_{\max} , RAQ10A0, RAQ10A1, RAQ10A2, RAQ10A3, CFALL, and VEGC2N, which are estimated based on conventional calibration.

evaluated in the context of sensitivity analyses [e.g., *Potter et al.*, 2001; *Knorr and Heimann*, 2001]. These sensitivity analyses are useful for biogeochemistry modelers to set the upper and lower bounds on simulations, and are often conducted by changing one parameter per simulation, and neglect the interactions among the parameters [e.g., *Potter et al.*, 2001; *Knorr and Heimann*, 2001]. Rather, the model parameters are often correlated [e.g., *Wang et al.*, 2006; Tang and Zhuang, submitted manuscript, 2008]. To consider the parameter correlations, *Ogle et al.* [2003] used Monte Carlo simulations by incorporating the information of probability density functions (PDFs) of the parameters and their covariance matrix into their analysis. However, the prior knowledge of parameter correlations is generally not readily available. Thus several researches constructed some statistical models based on regression between their biogeochemistry model outputs and parameters [*Tatang et al.*, 1997; *Ogle et al.*, 2007]. When a proper multivariate regression is performed, the output

from the statistical model will be close enough to the simulations from the process-based models. The uncertainty analysis was then conducted using the statistical model and the observed data [*Ogle et al.*, 2007]. These efforts are able to quantify regional uncertainty, in a first-order approximation, due to equifinality associated with the model parameters, but are not able to improve the model predictability as the uncertainty in parameters of the biogeochemistry model has not been constrained using any observed data, and higher-order contributions to the uncertainties in the outputs due to the nonlinear interactions among parameters are simply neglected.

[4] Model-data fusion techniques, such as, the Bayesian inference method, have been demonstrated to be able to quantify and constrain the uncertainty of model parameters and improve model predictability at site levels [e.g., *Trudinger et al.*, 2007; *Braswell et al.*, 2005; *Raupach et al.*, 2005; *Xu et al.*, 2006; *Williams et al.*, 2005; *Gove and Hollinger*, 2006; *Wang et al.*, 2001, 2007]. To apply these

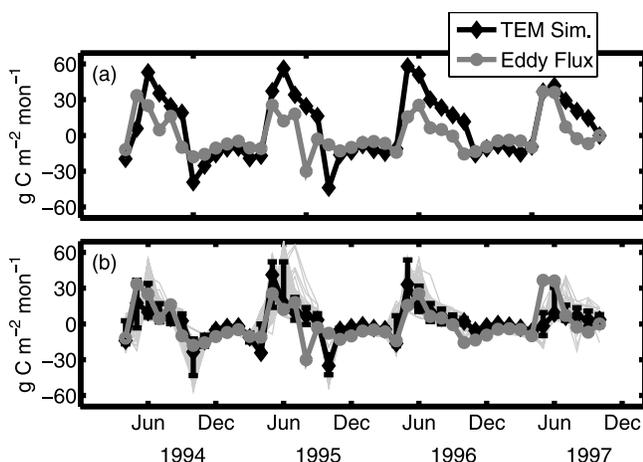


Figure 1. (a) TEM-simulated NEP with parameters from the conventional calibration. The linear regression model between the simulated NEP (dependent variables) and the observed data (independent variable) has $R^2 = 0.48$, slope = 0.40 ($p < 0.01$), intercept = $-2.47 \text{ g C m}^{-2} \text{ mo}^{-1}$, and root mean square error (rmse) = $20.7 \text{ g C m}^{-2} \text{ mo}^{-1}$. (b) The posterior TEM NEP after the Bayesian inference when all eddy flux data (measured NEP plus derived GPP and RESP) are used in the model-data fusion. The error bar denotes the 95% credible interval of the variables at that month; the black solid time series are the modes of distribution after the Bayesian inference. The linear regression model between the simulated NEP with “mode” parameters (dependent variables) and the observed data (independent variable) has $R^2 = 0.38$, slope = 0.72 ($p < 0.01$), intercept = $-0.52 \text{ g C m}^{-2} \text{ mo}^{-1}$, and rmse = $12.9 \text{ g C m}^{-2} \text{ mo}^{-1}$. Also shown in thin gray lines is NEP from every ensemble members composing the posterior NEP.

techniques to quantify uncertainties in estimates of regional carbon dynamics, *Knorr and Kattge* [2005] suggested that process-based biogeochemistry models should go through determination of parameters using the Bayesian techniques (e.g., using the Monte Carlo Markov Chain algorithm in their study) with the observed ecosystem flux data. The parameters and models could then be extrapolated to a region. Here we use a process-based biogeochemistry model, the Terrestrial Ecosystem Model (TEM; [*Melillo et al.*, 1993; *Zhuang et al.*, 2002, 2003]), site-level eddy flux tower data for a black spruce ecosystem, and a Bayesian inference framework (Tang and Zhuang, submitted manuscript, 2008), to conduct a such study. Our aim is to show that parameterization equifinality is a major uncertainty source to regional carbon estimates. We also show that using Bayesian techniques and process-based biogeochemistry modeling will provide more serious regional estimates of carbon dynamics and constrain their associated uncertainties.

2. Method

2.1. Overview

[5] We use the TEM and a Bayesian inference framework (Tang and Zhuang, submitted manuscript, 2008), to investigate how equifinality derived from site-level parameterization affects the uncertainty in the estimation of regional

carbon dynamics in boreal forest ecosystems (north of 45° N) during the 20th century. We parameterize TEM for boreal forest ecosystems at a black spruce forest ecosystem site [*Clein et al.*, 2002]. We first derive numerous sets of parameters for TEM with Bayesian techniques [*Zhuang et al.*, 2003; Tang and Zhuang, submitted manuscript, 2008]. We then conduct three groups of Monte Carlo simulations considering effects of parameterization equifinality and random noises in climate forcing. We also conduct TEM simulations with a set of parameters derived using conventional calibration techniques [e.g., *Raich et al.*, 1991; *McGuire et al.*, 1992]. The uncertainty in regional carbon dynamics estimation is characterized by presenting various statistics including mode and standard deviation from these simulations. Below, we first introduce the TEM model and the observed carbon flux data used in our Bayesian inference framework (Tang and Zhuang, submitted manuscript, 2008). Second, we describe how conventional and Bayesian methods have been applied to the parameterizations for the site and regional simulations with TEM. Finally, we describe the regional simulation protocol and how we characterize the uncertainty sources.

2.2. Terrestrial Ecosystem Model and Parameterizations

[6] TEM uses spatially referenced information on climate, elevation, soils, vegetation and water availability to make monthly estimates of vegetation and soil C and nitrogen (N) fluxes and pool sizes. The model is well-documented and has been used to examine patterns of regional and global terrestrial C dynamics [e.g., *Raich et al.*, 1991; *McGuire et al.*, 1992; *Melillo et al.*, 1993; *Zhuang et al.*, 2001, 2002, 2003; *McGuire et al.*, 2001]. The version of TEM used in this study explicitly couples biogeochemical processes with soil thermal dynamics of permafrost and non-permafrost soils [*Zhuang et al.*, 2001, 2002, 2003, 2006; *Euskirchen et al.*, 2006; *Balshi et al.*, 2006] and therefore is applicable to this region, dominated by boreal forest ecosystems. In TEM, the net ecosystem production (NEP), which is net carbon exchange between the land ecosystems and atmosphere, is calculated as the difference between the uptake of atmospheric CO_2 associated with photosynthesis (i.e., gross primary production or GPP) and the release of CO_2 through autotrophic respiration (R_A), heterotrophic respiration (R_H) associated with decomposition of organic matter. The fluxes GPP, R_A and R_H are influenced by changes in atmospheric CO_2 , climate variability and change, and the freeze-thaw status of the soil.

[7] We parameterize TEM with the conventional method at a mature black spruce ecosystem at Bonanza Creek, a Long-Term Ecological Research site in Alaska [*Zhuang et al.*, 2002]. The climate, vegetation, soil, and elevation for the site have been documented previously [*Zhuang et al.*, 2002]. In the conventional method, the parameters are obtained through manually adjusting the parameters controlling vegetation and soil carbon and nitrogen cycles [e.g., *Raich et al.*, 1991; *McGuire et al.*, 1992]. Specifically, the model continuously does integrations driven by long-term average climate data and atmospheric CO_2 concentrations of 340 ppmv. By changing parameter values, the simulated fluxes and pools sizes will match the field data with a certain tolerance (e.g., 1%), and then parameters values can

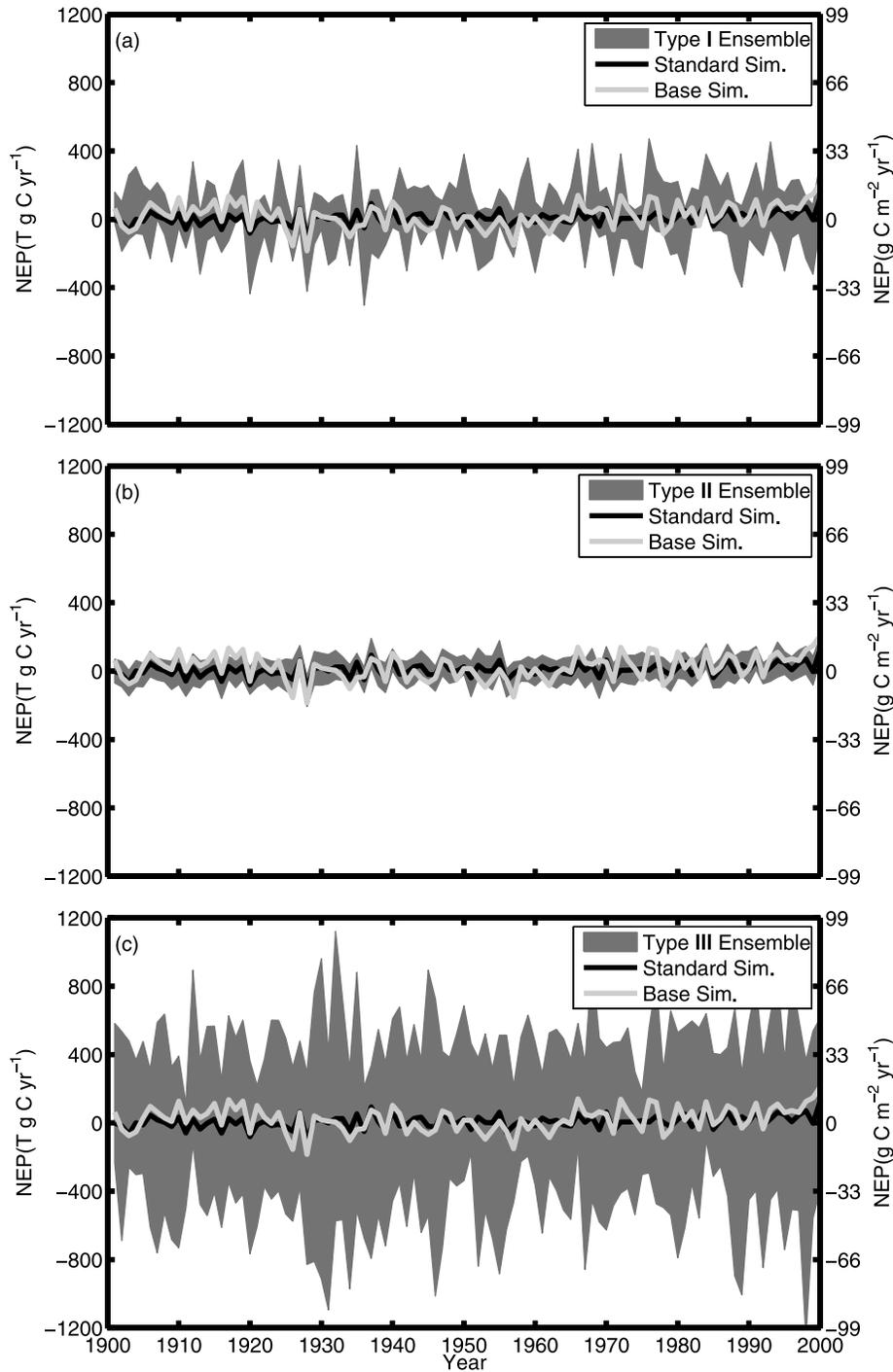


Figure 2. Annual NEP of the boreal forest ecosystem north of 45°N in the 20th century. Results from the ensemble simulations for (a) the type I uncertainty, (b) type II uncertainty, and (c) type III uncertainty.

be obtained. During the calibration, we will run TEM until (1) the modeled annual NPP and GPP match the observations, (2) the annual available nitrogen is close to the observations, and (3) the annual NEP converges to nearly zero with the tolerance specified above [Zhuang *et al.*, 2001; Clein *et al.*, 2002]. The set of parameters are considered optimal for the site (Table 1) and will be then used for regional extrapolations.

[8] To parameterize TEM with eddy flux tower data, we implement a Bayesian inference method to the Old Black

Spruce ecosystem in Northern Study Area (northern site, Manitoba, Canada) of BOREAS [Zhuang *et al.*, 2002; Clein *et al.*, 2002; Sellers *et al.*, 1997]. We adopt the following likelihood function (see Thiemann *et al.* [2001] for a detailed derivation and necessary assumptions)

$$p(\mathbf{V}|\boldsymbol{\theta}) = C \prod_{i=1}^N \left[\sum_{t=0}^T |v_i|^2 \right]^{(1/2-T)} \quad (1)$$

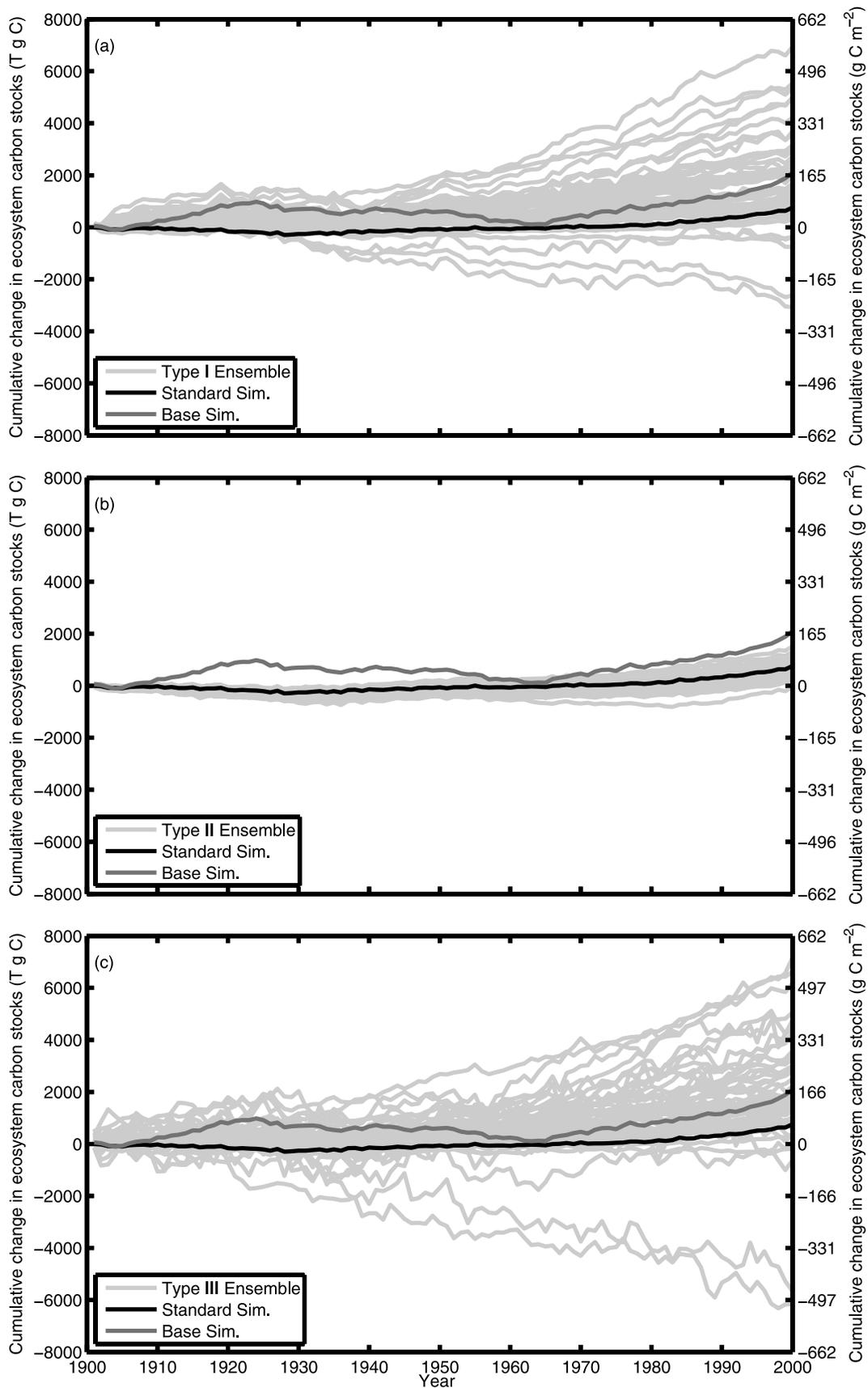


Figure 3. Cumulative change in ecosystem C stocks in boreal forest ecosystems north of 45°N in the 20th century. Results from ensemble simulations for (a) type I uncertainty, (b) type II uncertainty, and (c) type III uncertainty.

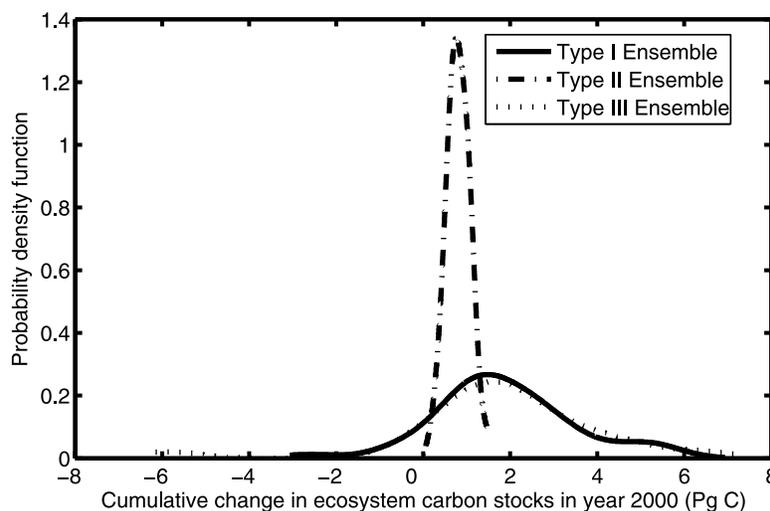


Figure 4. Probability density function of the cumulative changes in ecosystem C stocks in boreal forest by the end of 20th century due to three different types of uncertainty sources.

where \mathbf{V} is a vector containing the log-transformed observations, and $\boldsymbol{\theta}$ is a vector containing parameters to be inferred, and C is a normalizing constant, and N is number of different types of observations, and T is the total length of observations. The observed NEP and the other two deduced fluxes, GPP and RESP (i.e., ecosystem respiration, a sum of R_A and R_H), required in our Bayesian inference method are aggregated from half-hourly measurements to monthly time step for the period from 1994 to 1997 at the site [see *Clein et al.*, 2002]. In implementing the Bayesian inference, we use the sampling importance resampling (SIR) technique to draw the posterior from the prior TEM simulations [see *Skare et al.*, 2003]. We obtain a great number of sets of parameters, including a set of “mode” parameters, which have the highest plausibility (or best fitting with respect to observations) in the parameter space (Table 1). To derive these parameters, we assume that the prior parameters of TEM follow the uniform distributions with different ranges (see Table 1). The ranges are specified based on either literature review or our experience in calibrating TEM. On the basis of the prior distribution of the parameters, we sampled 150,000 sets of parameters using the Latin Hypercube Sampling technique (LHS; [Iman and Helton, 1988]) to conduct simulations at the site from 1975 to 1997. The Bayesian inference analyses are then conditioned on the eddy flux data of NEP.

[9] We now describe how to generate parameters for regional simulations by considering the equifinality deduced from the site-level parameterization. We first sample 150,000 sets of parameters from prior distributions of the parameters. We then filter those samples with available observations using the Bayesian inference technique described above. Finally we do a stratified sampling from these filtered parameters to obtain different sets of parameters for regional simulations. Our method implicitly considers the correlations among the parameters [Roulston and Smith, 2003]. Specifically, we obtain 50 sets of parameters with following steps:

[10] 1. A Bayesian inference procedure is performed onto the prior Monte Carlo ensemble simulations for the black

spruce forest ecosystem described above. The posterior NEP is thus obtained from 1994 to 1997 at a monthly time step (see Figure 1b).

[11] 2. Choose a simulated monthly NEP data point with the greatest uncertainty (i.e., the data point with the largest distance between its upper bound and the lower bound from the site-level ensemble simulations; for this study, we choose the data point in May 1994) and divide its uncertainty range into n segments with an equal probability, where n is the number of samples we want to generate. The NEP in each segment comes from simulations with different sets of parameters.

[12] 3. Randomly choose one point within each segment, and the set of parameters corresponding to such a chosen point is then used for one ensemble TEM simulation.

[13] 4. Repeat step III until n samples are collected.

[14] We set n as 50 for this study. These 50 sets of parameters are sampled in a stratified manner from the posterior NEP, thus are sufficient to reveal the regional uncertainty due to equifinality in parameterizations.

2.3. Regional Simulations

[15] Three types of TEM ensemble simulations are conducted, which consider: (1) the effect of equifinality associated with model parameterization (hereafter referred to as the type I uncertainty); (2) the uncertainty in climate forcing, including air temperature, cloudiness and precipitation, characterized by random noises (hereafter referred to as the type II uncertainty); and (3) both parameterization equifinality and random noises in climate forcing (hereafter referred to as the type III uncertainty). Our study spatial domain has total vegetated areas of 12.1 million km^2 in 7421 $0.5^\circ \times 0.5^\circ$ grid cells. In addition, we conduct a regional simulation with parameters obtained using the conventional calibration method [Zhuang et al., 2001, 2002]. We refer this simulation to as “Base Simulation” hereafter. To contrast the difference between the conventional calibration and the Bayesian inference method in regional simulations, we conduct another regional simulation with the set of “mode” parameters derived with the

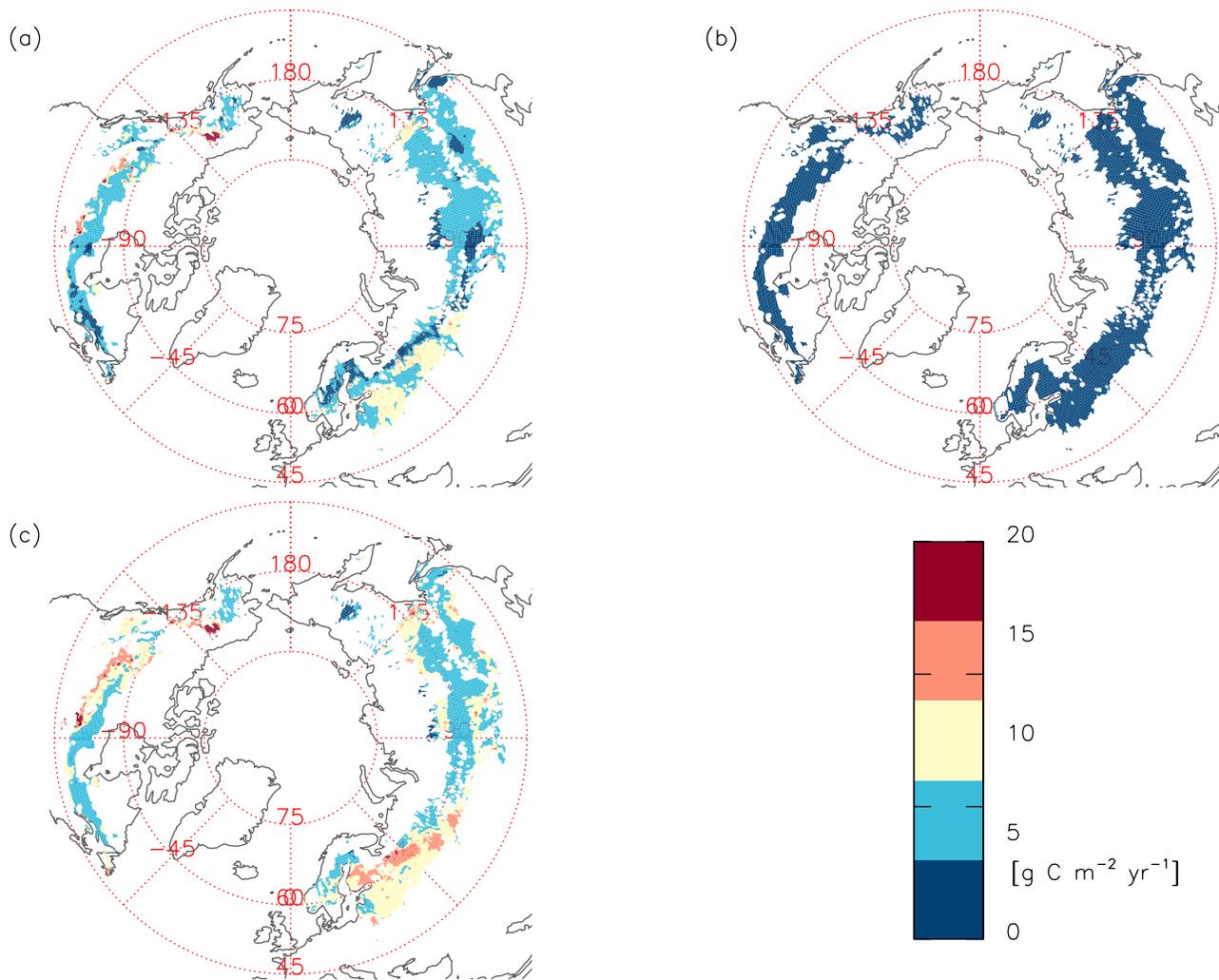


Figure 5. Comparison of spatial distributions of the standard deviation for the 1991–2000 decade when considering different types of uncertainties. (a) Type I uncertainty, (b) type II uncertainty, and (c) type III uncertainty.

Bayesian inference framework (Table 1). This simulation is hereafter referred to as “Standard Simulation”.

[16] To conduct the type I regional simulations, we run TEM with 50 sets of parameters derived using the method described above, but with the typical climate and atmospheric CO₂ data. To conduct the type II simulation, we perturb the air temperature, precipitation and cloudiness by imposing assumed random noises on each variable of the original CRU data [Mitchell *et al.*, 2004]. Specifically, the air temperature is perturbed from a -2°C decrease to a 2°C increase of original values, which is a reasonable assumption based on the study by Brohan *et al.* [2006]. The precipitation and cloudiness are perturbed from a decrease 15% to an increase 15% of original values. Such perturbations are applied from 1901 to 2000 for each month. For all the grid cells in a certain month of a certain year, same perturbations are imposed. We then randomly generate 50 sets of climate forcing data from those perturbations. The data are then used to drive ensemble simulations with the “mode” parameters derived from the Bayesian inference framework.

[17] The parameters and driving climate data sets for the type III ensemble simulations are derived from those for type I and type II ensemble simulations in a Latin hypercube sampling manner [Iman and Helton, 1988]. Specifically, they are generated by randomly pairing the set of parameters for i -th member simulation of type I ensemble to the climate forcing data set for j -th member simulation of type II ensemble. Such a treatment assumes the parameter samples and the driving climate data samples are independent from each other. As a result, we conduct another 50 regional simulations with 50 sets of parameters and forcing data.

[18] For all these regional simulations, we first run the model to equilibrium (i.e., annual NEP is close to zero) with the long-term mean climate from 1901 to 2000. We then spin up the model for 120 years with the first 40 years climate data. The model is then run starting from 1901 to 2000 with the transient climate data for each grid cell.

3. Results

[19] The site-level simulation with conventional calibration is different from the posterior NEP inferred through

Table 2. Comparisons of 10-year Average (1991–2000) NEP in Different Continents With Units of Tg C yr^{-1a}

Continents	North America	Europe	Northern Asia
Base Simulation	46.8 (13.2)	15.0 (5.6)	33.0 (5.6)
Standard Simulation	17.7 (5.0)	11.8 (4.4)	14.5 (2.5)
Type I ensemble	17.4 (4.9) ± 15.2 (4.3)	7.1 (2.6) ± 10.3 (3.8)	15.7 (2.7) ± 20.9 (3.6)
Type II ensemble	17.7 (5.0) ± 2.0 (0.6)	12.4 (4.6) ± 2.0 (0.7)	16.4 (2.8) ± 3.1 (0.5)
Type III ensemble	17.3 (4.9) ± 19.4 (5.5)	10.9 (4.0) ± 18.4 (6.8)	17.5 (3.0) ± 27.5 (4.7)

^aThose in brackets are area-averaged values with units of g C m⁻² yr⁻¹.

Bayesian inference (Figure 1). This difference is resulted from different assumptions in model parameterization. The parameterization equifinality does occur in TEM (Figure 1b). TEM is able to reproduce the observed NEP with certain uncertainty using different sets of parameters, but the same external forcing.

[20] Below, we first summarize the sources to the inter-annual uncertainty of the estimated carbon dynamics in the region. To compare different sources, the nonparametric estimation of the probability density functions (PDFs) for carbon storage is derived for all three types of uncertainty ensemble simulations [Vikas and Duraiswami, 2006]. We then show how different uncertainty sources influence the estimation of spatial carbon dynamics using the average NEP in the 1990s. The spatial patterns of NEP derived from the ensemble simulations, the Standard Simulation, and the Base Simulation are compared. Finally we identify the major uncertainty sources of seasonal carbon dynamics in the region. The uncertainty in simulated carbon fluxes is referred to their magnitudes, except stated otherwise.

3.1. Uncertainty Sources in Estimating Carbon Storage During the 20th Century

[21] Between random noises in climate forcing and the equifinality of the parameters, the latter is a larger uncertainty source to the estimation of carbon sequestration in the region (Figure 2). When both equifinality and random noises in climate forcing are considered, the type III ensemble simulations show the largest uncertainty range because of the multiplicative effects of these two uncertainty sources (Figure 2c). The inter-annual NEP in the Base Simulation and the Standard Simulation are different in both their phases and amplitudes (Figure 2). As a result, the cumulative changes in ecosystem carbon stocks from these two simulations are different. Specifically, in the Base Simulation, after a short nearly neutral period, the NEP first shows a steady increase until 1924 then an irregular decrease until 1963 and then another steady increase until 2000. In contrast, in the Standard Simulation, NEP shows a very steady but small increase after a long nearly neutral or weak source period until 1970, and then becomes a small sink until 2000 (Figure 3). The PDFs of the cumulative

change in ecosystem carbon stocks also indicate that the type II ensemble simulations have sharper convergence, while type I and type III ensemble simulations provide more dispersive convergences (Figure 4). The parameterization equifinality provides a larger span of simulations than that due to random noises in climate forcing for the carbon storage (Figure 4). Given the uncertainty in both parameters and climate forcing data, the TEM simulations indicate that the boreal forest ecosystems are a C sink ranging from 0.7 to 2.5 Pg C, while the Base Simulation estimates 2.1 Pg C and the Standard Simulation estimates 0.76 Pg C by the end of the 20th century (see Figures 3 and 4). This suggests that the equifinality of parameterizations at a site will result in diverged estimates of regional carbon dynamics using TEM during the 20th century.

3.2. Uncertainty Sources in Estimating Spatial Carbon Dynamics

[22] By comparing the spatial pattern of the standard deviation derived from the three types of ensemble simulations from 1991 to 2000, we find that the parameterization equifinality is also an overwhelming uncertainty source to the estimate of spatial carbon dynamics (Figure 5). The mean decadal carbon storage varies depending on uncertainty sources and parameterization methods (Table 2). Specifically, North America acts as a carbon sink ranging from 17.3 to 46.8 Tg C yr⁻¹ with large uncertainty, while Europe's sink ranges from 7.1 to 15 Tg C yr⁻¹ and Northern Asia acts as a sink between 14.5 to 33.0 Tg C yr⁻¹ during this 10-year period. On a per unit area basis, the large uncertainty also exists in these regions (Table 2). Overall, these simulations indicate that the large areas of North America are mostly a C sink during the period, while Europe and Northern Asia act as a weaker C sink or neutral (Table 2 and Figure 5). The uncertainties associated with these estimates are significantly different in these regions with a large uncertainty in Europe and a relatively small uncertainty in North America. These discrepancies may be related to different sensitivities of TEM to parameters in different regions. In addition, the parameterization based only on a black spruce forest ecosystem in North America may also contribute to the discrepancies. On the basis of the

Table 3. Comparisons of 10-year Average (1991–2000) NEP in Different Continents at Probability of 66% and 90%, With Units of Tg C yr^{-1a}

	66%			90%		
	North America	Europe	Northern Asia	North America	Europe	Northern Asia
Type I ensemble	≤27.3 (7.7)	≤14.5 (5.4)	≤29.4 (5.0)	≤52.0 (14.7)	≤35.0 (13.0)	≤61.6 (10.5)
Type II ensemble	≤21.3 (6.0)	≤15.0 (5.6)	≤22.8 (3.9)	≤29.4 (8.3)	≤21.9 (8.1)	≤36.5 (6.2)
Type III ensemble	≤28.9 (8.2)	≤18.4 (6.8)	≤34.2 (5.8)	≤61.1 (17.2)	≤48.2 (17.9)	≤78.7 (13.4)

^aThose in brackets are area-averaged values with units of g C m⁻² yr⁻¹.

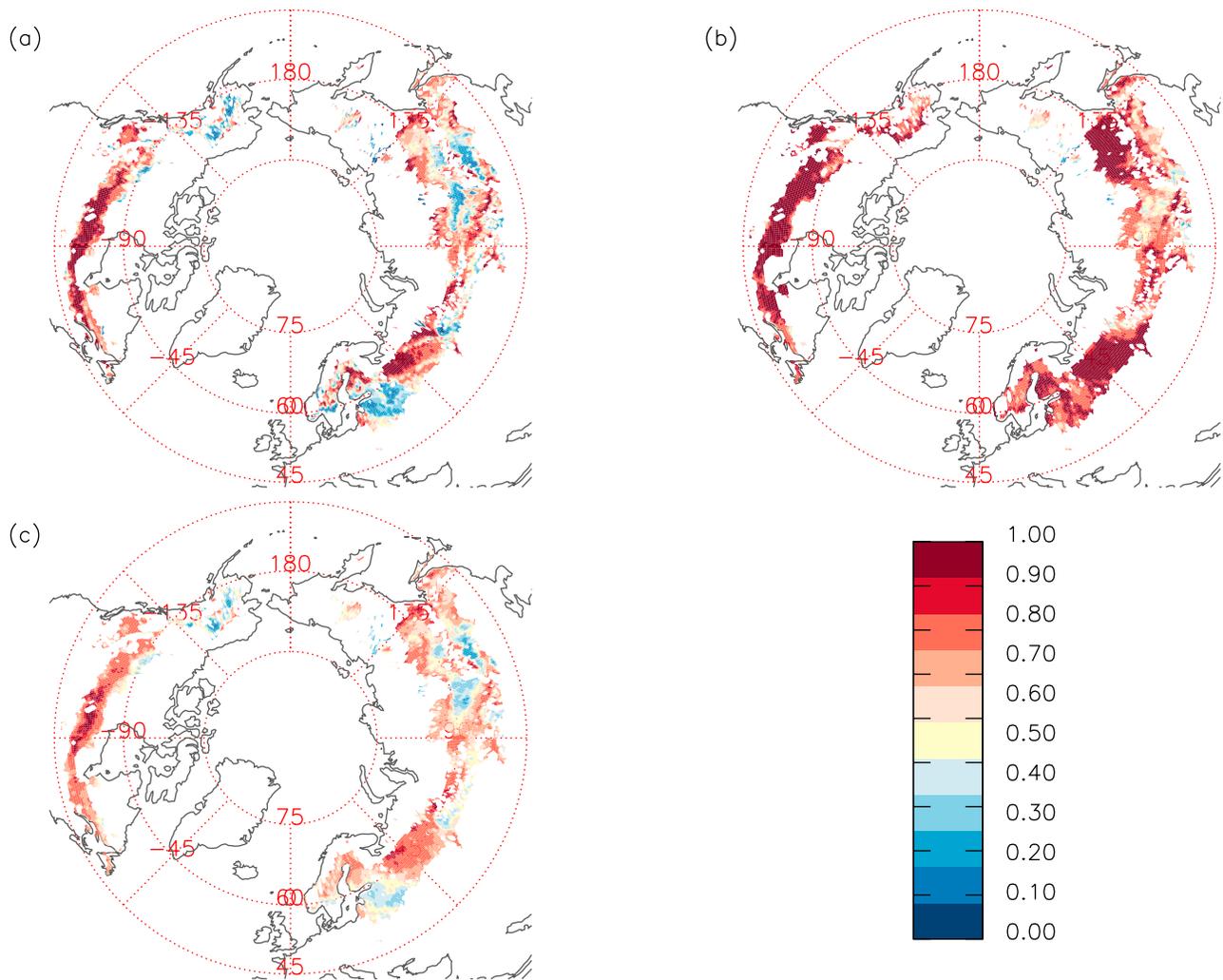


Figure 6. Spatial distributions of the probability as a carbon sink during 1991–2000. Results from ensemble simulations for (a) type I uncertainty, (b) type II uncertainty, (c) type III uncertainty.

ensemble simulations, we further obtained the sink values at 66% and 90% probabilities, which are defined as “likely” and “very likely”, respectively. We find that the North America likely acted as a carbon sink between 21.3 and 27.3 Tg C yr⁻¹ while Europe between 14.5 and 18.4 and Northern Asia between 22.8 and 29.4 Tg C yr⁻¹. Three regions acted very likely as a carbon sink ranging from 29.4 to 52.0 Tg C yr⁻¹, from 21.9 to 48.2 Tg C yr⁻¹, and from 36.5 to 78.7 Tg C yr⁻¹ for North America, Europe and Northern Asia, respectively (Table 3). These analyses suggest that uncertainty in characterizing regional carbon sink or source strengths resulted from parameterization equifinality and random noises in climate forcing varies spatially.

[23] By further calculating the ratio of the members with positive NEP among the 50 ensemble members, we contour the probability for grid cells to be a carbon sink in the 1990s (Figure 6). Majority of grid cells in North America acts as a C sink during this period, no matter what type of uncertainty is considered. When the parameters are uncertain such as in type I and type III ensemble simulations, a large portion of Northern Asia and Europe appears more likely to be carbon sources (Figures 6a and 6c). When only the type II uncertainty is considered, the whole boreal forest ecosystem appears very likely as a C sink, except in some parts of northern Asia. We summarize the statistics related to these sink and source activities in Table 4, where the relative areas

Table 4. Comparisons of Relative Sink Areas at the Threshold Probabilities of 66% and 90% in Different Continents During the Period from 1991 to 2000

	66%			90%		
	North America	Europe	Northern Asia	North America	Europe	Northern Asia
Type I Ensemble	72.5	53.8	58.0	47.6	36.0	30.5
Type II Ensemble	97.1	98.3	80.8	81.5	87.2	52.2
Type III Ensemble	73.5	61.6	57.4	30.5	17.7	14.5

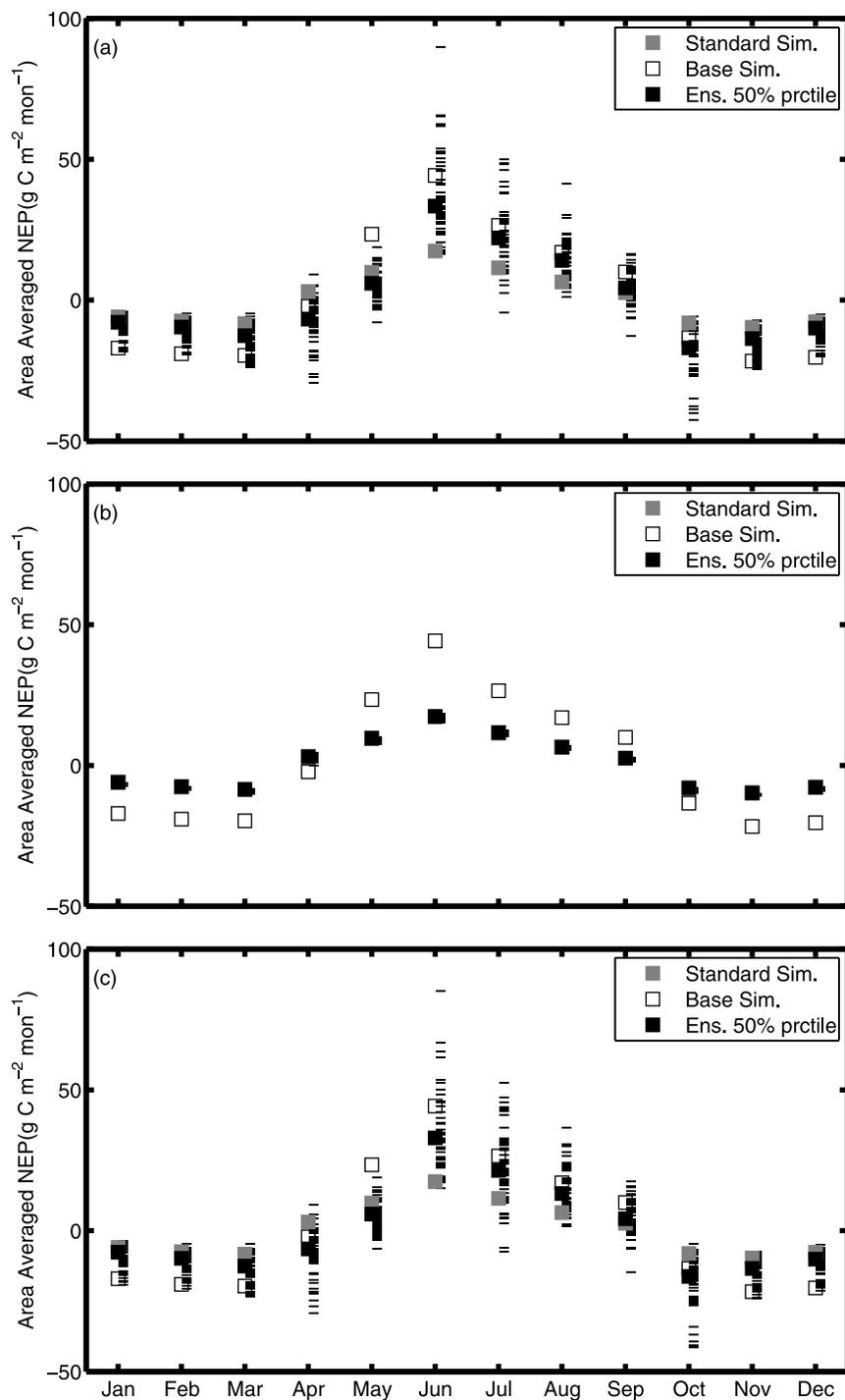


Figure 7. Decadal mean (1991–2000) of area-averaged seasonal NEP patterns due to different types of uncertainty. (a) Type I uncertainty, (b) type II uncertainty, and (c) type III uncertainty. The minus signs are NEP from ensemble members. The ensemble 50th percentile (Ens. 50% prctile) is computed using the prctile function in Matlab v7.3.0.267.

as a C sink in all three continents are presented at both 66% and 90% probabilities. We conclude that, at least more than 70% of North American boreal forests act likely as a C sink, no matter what type of uncertainty is accounted. In contrast, the northern Asia is the least productive among three continents with the “very likely” values between 14.5 and 52.5%, while North America and Europe have the values of

30.5–81.5% and 17.7–87.2%, respectively. These analyses suggest that the equifinality and climate forcing will also affect the estimate of C sink areas in these continents.

3.3. Uncertainty Sources in Estimating Seasonal Carbon Dynamics

[24] In a site-level study, we showed that the seasonal C dynamics in a black spruce forest ecosystem depend criti-

Table 5. Decadal Mean (1991–2000) of Area-Averaged NEP ($\text{g C m}^{-2} \text{yr}^{-1}$) Simulated with CRU Data and NCEP/NCAR Global Reanalysis Data and Cumulative Changes in Ecosystem C Stocks (CCECS, unit: Tg C) by the End of the 20th Century Simulated with CRU Data (1901–2000) from the Single-Variable Sensitivity Simulations^a

	Standard Simulation	Tair +2°C	Tair -2°C	Clds +15%	Clds -15%	Prec +15%	Prec -15%
NEP (CRU 1991–2000)	3.6	3.9	3.3	3.9	4.2	4.0	4.6
NEP (NCEP 1991–2000)	1.33	1.02	0.85	1.31	1.34	1.29	1.31
CCECS at 2000 with CRU data from 1901–2000	763.0	964.6	386.6	777.0	961.3	786.7	1096.0

^aTair, Clds, and Prec represent air temperature, cloudiness, and precipitation, respectively.

cally on the parameters used, including both their values and correlations (Tang and Zhuang, submitted manuscript, 2008). For instance, we found that, the same amount of variation of parameter CMAX, the maximum rate of photosynthesis C, results in 10% of the variation of NEP in May, but increases NEP sink by 30% in June, then decreases NEP sink less than 10% in September. When these fluctuations resulted from parameterization equifinality are extrapolated to a region, the uncertainty of the decadal NEP widely spans in the growing season from April to October (Figures 7a and 7c). The uncertainty is large in June, and has different distribution shapes from one month to another. In contrast, the random perturbation of the driving climate data does not significantly impact NEP (see Figure 7b).

[25] A larger seasonal difference exists in May, June and July, and a relatively smaller difference in April and October (Figure 7). In other months, the differences are almost same from one simulation to another. When such magnitude differences in the seasonal C dynamics are integrated with time, the multi-decadal differences between the NEP simulated in the Base Simulation and the Standard Simulation are dramatic (Figure 3). Such differences are more evident in the cumulative changes in ecosystem C stocks (Table 5). These analyses suggest that the seasonal uncertainty influenced by equifinality is a key uncertainty source to the inter-annual uncertainty in the region.

4. Discussion

[26] In this study, we show that, given the same model structure and climate forcing being used, the equifinality [Beven and Freer, 2001] of the parameters (type I uncertainty) results in a much larger uncertainty to the simulated C dynamics than that due to random noises in climate data (type II uncertainty). Below we first further contrast the uncertainty sources between parameterization equifinality and random noises in climate data by conducting a set of sensitivity analyses based on CRU data [Mitchell et al., 2004] and NCEP/NCAR global reanalysis data [Kistler et al., 1999]. Second, we will compare the influence between parameterization equifinality and the uncertainty of model structures on regional uncertainty. Third, we will discuss how regional uncertainty will be influenced by the uncertainty at different temporal and spatial scales. Fourth, we briefly discuss the usefulness of our method presented in this study in improving estimates of regional carbon dynamics. Finally, we discuss factors and processes we have not considered in this analysis.

[27] First, in the type II uncertainty simulations, we do not increase or decrease all data for a certain variable with the same magnitude as did in the study of Potter et al. [2001]. Rather, we assume the climate data set used is only

subject to random noises. We thence perturb them using a uniform distribution specified by some lower and upper bounds of changes and a random pairing procedure. As a result, the uncertainty resulted from these perturbations tends to be narrower (Figure 2). To test if the uncertainty type II has been underestimated in regional simulations, we conduct a set of single-variable sensitivity simulations by altering one variable at a time. Our results show that there are small or moderate changes in both area-averaged NEP and total C accumulation by the end of 20th century before and after perturbations (Table 5). When different climate data sets were used, a recent study indicated that the uncertainty in carbon sequestration estimation could be much larger [Clein et al., 2007]. This is consistent with our results based on simulations with the NCEP/NCAR global reanalysis data (Table 5). However, the results based on NCEP/NCAR data also showed small changes in NEP in all sensitivity simulations. This suggests that the parameterization equifinality will result in a larger uncertainty in comparison to the effect of random noises in climate forcing no matter which climate data set is used.

[28] Second, to contrast the effect of parameterization equifinality and uncertain model structures on regional uncertainty, we compare our regional average NEP with site-level results simulated with multiple models by Amthor et al. [2001]. When the type I and III uncertainty is considered, our regional NEP varies from -6.7 to $10.8 \text{ g C m}^{-2} \text{yr}^{-1}$ for the type I uncertainty and from -10.9 to $15.7 \text{ g C m}^{-2} \text{yr}^{-1}$ for the type III uncertainty in the 1990s. Using nine models, Amthor et al. [2001] found the baseline NEP varies from -11 to $61 \text{ g C m}^{-2} \text{yr}^{-1}$ in year 1996 for the black spruce ecosystem that we used for parameterization. This comparison suggests that the uncertainty due to different parameterizations in our simulations is comparable with the uncertainty due to different model structures, which is another source that contributes to the uncertainty in modeling regional C dynamics.

[29] Third, we show that the uncertainty in the simulated C dynamics varies temporally and spatially. These uncertainty structures depend more on parameterization equifinality than on random noises in climate data. For instance, with the same driving climate data, the NEP produced by the Base Simulation shows a significant multi-decadal variation, which accordingly results in significant multi-decadal variations in cumulative changes of ecosystem C stocks, whereas no such significant multi-decadal variation is found in the Standard Simulation (see Figures 2 and 3). This suggests that, if we attribute C dynamics simulated with the same set of parameters to variations in climate, while excluding the possible causes by large uncertainty in parameters, we may seriously bias the regional estimates. Similarly, conducting a few simulations with the same set of

parameters may seriously bias the estimates of spatial distributions of C dynamics. For example, the Base Simulation shows that Europe and northern Asia have almost equal NEP during the 1990s, but the Standard Simulation shows the Europe has much larger NEP. In addition, when the seasonal C dynamics are considered, their uncertainty shows a strong seasonal-dependence. Uncertainty is greater in the growing season and less in the non-growing season. Such a seasonal-dependence was also found in the nine-model comparison study by Amthor *et al.* [2001]. We conceive such behavior in the uncertainty of modeling seasonal carbon dynamics is related to the poor constraint on the parameterizations and formulations of the growing season dynamics. As showed by Tang and Zhuang (submitted manuscript, 2008), the simulated carbon fluxes are most sensitive to these parameterizations in the growing season. If they are otherwise well constrained, the uncertainty behavior should agree with the eddy-flux measurement in NEP, which shows a less uncertainty in the growing season rather than in the non-productive season [Raupach *et al.*, 2005]. These comparisons suggest that the parameterization equifinality needs to be considered when conducting both seasonal and inter-annual estimates of carbon dynamics in the region.

[30] Fourth, while we show that the parameterization equifinality is a significant source to the estimate of carbon dynamics, we also indicate that, to reduce the uncertainty of regional simulations using process-based biogeochemistry models, applying Bayesian inference techniques with observed flux data in a biogeochemistry model-data fusion fashion is a vital approach. To improve biogeochemistry model parameterizations at site-levels, a number of calibration or parameter estimation methods are available [e.g., Raupach *et al.*, 2005; Trudinger *et al.*, 2007]. To improve regional estimates, we suggest multi-site calibration methods could be attempted. For example, merging methods including spatial Bayesian model average algorithm [Berrocal *et al.*, 2007] and the Bayesian multi-model merging algorithm [Luo *et al.*, 2007] are promising. These methods assume that each set of parameters or model formulation is able to reproduce the observation with certain accuracy. All sets of parameters or model formulation together with their associated uncertainties expressed in probability will give a better representation of the ecosystem dynamics. In this context, our study is a first step in developing regional estimates using observed data at site-levels and process-based biogeochemistry models.

[31] Finally, there are many other uncertainty sources that we have not considered in this analysis. They include effects of different model structures, fire disturbances [Zhuang *et al.*, 2002; Balshi *et al.*, 2006], deforestation and nutrient fertilization [McGuire *et al.*, 1997]. In addition, insect outbreak is another significant disturbance that has not been accounted for [Kurz *et al.*, 2008]. These factors should be taken into account in future uncertainty analysis.

5. Conclusion

[32] Simple extrapolation with a set of parameters deduced from a site-level calibration to a region is a traditional way to estimate regional carbon dynamics. This procedure could result in severe biases to regional estimates. In this study, using the process-based biogeochemistry model TEM and

a Bayesian inference framework, we show that the equifinality in site-level parameterizations is an overwhelming uncertainty source to the estimates of regional carbon dynamics in boreal forest ecosystems during the 20th century. We further demonstrate that the uncertainties associated with parameterization equifinality vary both spatially and seasonally. Our study indicates that, to make a more serious estimation of regional C dynamics, Monte Carlo ensemble simulations constrained with the observed data using biogeochemistry models and Bayesian inference techniques should be conducted.

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