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Simple models for soil CO_2, CH_4, and N_2O fluxes calibrated using a Bayesian approach and multi-site data

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ABSTRACT

Emissions and uptake of soil greenhouse gases (GHG) are controlled by soil biogeochemical processes. We developed simple models, which were termed SG models, for soil CO_2 efflux, CH_4 uptake, and N_2O efflux in forest soils. We described each gas flux in terms of three functions: soil physiochemical properties (C/N ratio for CO_2 and N_2O, bulk density for CH_4; 0–5-cm soil layer), water-filled pore space (WFPS, 5-cm depth) and soil temperature (5-cm depth). Multi-site data, which were gathered monthly in Japanese forests over 3 years, were used for model calibration (36 sites, $n = 768$ in total for each gas flux). We used Bayesian calibration for optimization of the models. The functions for soil physiochemical properties were as follows. As soil C/N ratio increases, CO_2 flux increases, but N_2O flux rapidly decreases. CH_4 uptake decreases with increasing bulk density. Calibration clearly revealed the different sensitivities of each gas flux to WFPS and soil temperature. The estimated optimum WFPS for CO_2 flux was around 0.5 (intermediate), whereas CH_4 flux decreased with increasing WFPS, and N_2O flux increased with increasing WFPS. The Q_{10} values for CO_2, CH_4, and N_2O fluxes were 1.9, 1.1, and 3.4, respectively. Our models reproduced observed GHG fluxes well, both in comparison to each observation and the site average. The SG models require only three inputs, which are easily measurable and are therefore suitable for regional application and incorporation into other models as GHG submodels.

1. Introduction

CO_2, CH_4, and N_2O are major greenhouse gases (GHG) (IPCC, 2007), and forest soils play an important role in the emissions of CO_2 and N_2O and the uptake of CH_4 (except for anaerobic soils). These gas fluxes are controlled by soil physiochemical properties, temperature, and soil water conditions (Ishizuka et al., 2002; Davidson et al., 2004; Butterbach-Bahl et al., 2004; Morishita et al., 2004).

Modeling is a useful tool for tracing detailed processes, estimating regional GHG fluxes, and also predicting changes in the fluxes that will be caused by climate change (Potter et al., 1996; Del Grosso et al., 2005). A number of process-oriented models have been proposed for the evaluation of GHG emissions/uptake (e.g., Li et al., 2000). Because these models include complex processes involving carbon, nitrogen, and water, they require many inputs (e.g., daily climate data, like maximum and minimum temperature, precipitation, and solar radiation, and detailed soil physiochemical and vegetation properties) and include dozens or hundreds of parameters. These models are developed for tracing detailed processes and are suitable for application at sites that have enough input data and for use in investigating detailed processes. Whereas simpler models cannot trace such detailed processes, they are essential for regional applications or incorporation into other models. Simpler models require fewer inputs and are easier to handle (e.g., a soil carbon model by Liski et al., 2005). Furthermore, they also have the advantage that the link between input variables and output is clear and easy to evaluate.

One of the keys when building models is determination of the data used for parameterization; the reliability of a model is higher when the model is parameterized using a wider range of data (e.g., many sites, many kinds of vegetation and/or soil types, and interannual variations). Particularly when we apply the model to the regional scale, the parameterization should be conducted using a wider range of data for more accurate and precise estimates.

In this study, we constructed simple models for soil CO_2 efflux, CH_4 uptake, and N_2O efflux that are suitable for use in regional evaluation and for incorporation into other models. Each model calculates gas flux as a function of soil physiochemical properties, water-filled pore space (WFPS), and soil temperature. The input variables required are C/N ratio (0–5-cm soil layer) for the CO_2 and N_2O models, bulk density (0–5-cm depth) for the CH_4 model, WFPS (5-cm depth), and soil temperature (5-cm depth).

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For parameterization, we used multi-site data observed monthly in Japanese forests over 3 years (36 sites, $n = 768$ for each gas flux). We applied a Bayesian calibration scheme (Van Oijen et al., 2005), which is an optimization scheme that uses Monte Carlo sampling (Van Oijen et al., 2005; Müller et al., 2007), and is the best available scheme for estimating best-fit parameters based on observation data. In particular, the method has often been used for seeking universal parameters against multi-site datasets (Lehuger et al., 2009; Tuomi et al., 2009). The method also provides for the uncertainty of estimated parameters. The use of this method has been steadily increasing (Bates and Campbell, 2001; Xu et al., 2006; Tuomi et al., 2009; Lehuger et al., 2009; Yeluripati et al., 2009).

The purposes of this study were (1) to construct simple models for CO_2, CH_4, and N_2O fluxes; (2) to calibrate the models with multi-site field observation data from Japanese forest soils using the Bayesian calibration scheme; and (3) to evaluate the differences in the responses of each gas flux to soil water and temperature through parameterization.

2. Materials and methods

2.1. Model structure

We developed Simple greenhouse Gas models, which we termed SG models. In these models, each gas flux (CO_2, $\mu g\,C\,m^{-2}\,s^{-1}$; CH_4, $\mu g\,C\,m^{-2}\,h^{-1}$; and N_2O, $\mu g\,N\,m^{-2}\,h^{-1}$) is described by the same three factors: soil physiochemical properties, soil water, and soil temperature:

$$\text{Gas flux} = f(\text{SP})g(\text{WFPS})h(T) \tag{1}$$

where f(SP) is the function for soil physiochemical properties (SP, 0–5-cm soil layer), g(WFPS) is the function for WFPS (5-cm depth), and $h(T)$ is the function for soil temperature (5-cm depth). We adopted this simple structure because the goal of this study was to build simple models. We used one soil physiochemical property for each gas flux, and the variable was chosen after plotting various variables with the data and examining published papers.

The function for soil physiochemical properties was described using an exponential function with parameters m and n in common. The function for CO_2 flux was defined to increase with increasing C/N ratio (CNR, 0–5-cm soil layer):

$$f(\text{CNR}) = me^{n\text{CNR}} \tag{2}$$

The function for CH_4 flux was defined to decrease with increasing bulk density (BD, $Mg\,m^{-3}$, 0–5-cm soil layer):

$$f(\text{BD}) = me^{-n\text{BD}} \tag{3}$$

For N_2O flux, the function was defined to decrease with decreasing CNR:

$$f(\text{CNR}) = me^{-n\text{CNR}} \tag{4}$$

As for CO_2, the function was determined after plotting flux data against C concentration (%), content ($Mg\,m^{-3}$), and C/N ratio. Although the correlation was weak, we found that the C/N ratio was more closely correlated with the CO_2 flux than with the other gas fluxes. We then tested both a linear function (mCNR + n) and an exponential function (mCNR^n) and found that the exponential function performed slightly better. As for the CH_4 and N_2O fluxes, the functions were determined by examining published papers (CH_4: Ishizuka et al., 2009; N_2O: Nishina et al., 2009a,b).

The function for WFPS (5 cm) was defined by the following equation and used for every gas model:

$$g(\text{WFPS}) = \left(\frac{\text{WFPS} - a}{b - a}\right)^d \left(\frac{\text{WFPS} - c}{b - c}\right)^{-d((b-c)/(b-a))} \tag{5}$$

where a, b, c, and d are the parameters. The function has a convex shape, and values range from 0 to 1. The parameters a and c are the minimum and maximum values of WFPS, respectively (i.e., $g(a) = g(c) = 0$). The parameter b, which ranges between a and c, is the optimum parameter (i.e., $g(b) = 1$). The parameter d controls the curvature of the function, but the three other parameters also affect the shape. This function was adopted from the DAYCENT model (Parton et al., 1996; Del Grosso et al., 2000). Because the data we used in this study did not include WFPS, WFPS was calculated as a function of measured bulk density (BD, $Mg\,m^{-3}$, 5 cm) and volumetric soil water content (θ, 5 cm) using the following equation (Parton et al., 2001):

$$\text{WFPS} = \frac{\theta}{\left(1 - (\text{BD}/2.65)\right)} \tag{6}$$

The exponential function was used for the soil temperature for every gas flux. The equation is as follows:

$$h(T) = e^{pT} \tag{7}$$

where p is the parameter, and T is soil temperature (°C, 5 cm). $h(T)$ is 1 when the soil temperature is 0 °C.

The seven parameters of the model, two for the function of soil physiochemical properties (m, n), four for the function of WFPS (a, b, c, d), and one for the function of soil temperature (p), were determined using Bayesian calibration (see below).

2.2. Bayesian calibration

2.2.1. Bayes' theorem

Bayesian calibration is a model calibration method (Van Oijen et al., 2005; Müller et al., 2007) based on Bayes' theorem. Bayes' theorem is described in the following equation:

$$pr(\theta|x) = \frac{pr(\theta)pr(x|\theta)}{pr(x)} \tag{8}$$

where x is the observation, θ is the parameter, $pr(\theta|x)$ is the conditional probability of θ on x or the posterior distribution of θ, $pr(\theta)$ is the prior probability of θ, $pr(x|\theta)$ is the conditional probability of observations x on θ, and $pr(x)$ is the probability of observation x. The equation can be written in the following form:

$$pr(\theta|x) \propto pr(\theta)pr(x|\theta) \tag{9}$$

In general, a Gaussian function is assumed for the error function, $pr(x|\theta)$ (Van Oijen et al., 2005; Xu et al., 2006; Müller et al., 2007), and the posterior function can be written as follows:

$$pr(\theta|x) \propto pr(\theta)\prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-(x_o - x_m)^2/(2\sigma^2)} \tag{10}$$

where x_o and x_m are the measured and modeled values, respectively, n is the number of data points, and σ is the standard deviation. We assumed a uniform distribution, $U(\theta_{min}, \theta_{max})$, for each parameter:

$$pr(\theta_1) = 0 \text{ for } \theta_1 < \theta_{min} \text{ or } \theta_1 > \theta_{max} \tag{11}$$

$$pr(\theta_1) = \frac{1}{\theta_{max} - \theta_{min}} \text{ for } \theta_{min} \le \theta_1 \le \theta_{max} \tag{12}$$

where θ_1 is a parameter, and θ_{min} and θ_{max} are the lower and upper boundaries of the uniform distribution. In practice, calculations were performed in logarithms because it was computationally easier. The observed standard deviation for each gas flux was used for σ in this study.