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### The effects of constraining variables on parameter optimization in carbon and water flux modeling over different forest ecosystems



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#### ABSTRACT

The ability of terrestrial biogeochemical models in predicting land-atmospheric carbon and water exchanges is largely hampered by the insufficient characterization of model parameters. The direct observations of carbon/water fluxes and the associated environmental variables from eddy covariance (EC) flux towers provide a notable opportunity to examine the underlying processes controlling carbon and water exchanges between terrestrial ecosystems and the atmosphere. In this study, we applied the Metropolis simulated annealing technique to conduct parameter optimization analyses of a processbased biogeochemical model, simplified PnET (SIPNET), using a variety of constraining variables from EC observations and leaf area index (LAI) from MODIS at three ChinaFLUX forest sites: a temperate mixed forest (CBS), a subtropical evergreen coniferous plantation (QYZ) and a subtropical evergreen broadleaved forest (DHS). Our analyses focused on (1) identifying the key model parameters influencing the simulation of carbon and water fluxes with SIPNET; (2) evaluating how different combinations of constraining variables influence parameter estimations and associated uncertainties; and (3) assessing the model performance with the optimized parameterization in predicting carbon and water fluxes in the three forest ecosystems. Our sensitivity analysis indicated that, among three different forest ecosystems, the prediction of carbon and water fluxes was mostly affected by photosynthesis-related parameters. The performances of the model simulations depended on different parameterization schemes, especially the combinations of constraining variables. The parameterization scheme using both net ecosystem exchange (NEE) and evapotranspiration (ET) as constraining variables performed best with most well-constrained parameters. When LAI was added to the optimization, the number of well-constrained model parameters was increased. In addition, we found that the model cannot be well-parameterized with only growingseason observations, especially for those forest ecosystems with distinct seasonal variation. With the optimized parameterization scheme using both NEE and ET observations all year round, the SIPNET were able to simulate the seasonal and inter-annual variations of carbon and water exchanges in three forest ecosystems.

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#### 1. Introduction

In recent years, a large number of observations of landatmospheric carbon and water exchanges between terrestrial ecosystems and the atmosphere have been accumulated, mainly

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from environmental control experiments, eddy covariance (EC) measurements and remote sensing monitoring (Baldocchi et al., 2001; Stockli et al., 2008; Zhang et al., 2009; Williams et al., 2009). As the experiments and measurements are often conducted at limited sites and on specific scales, it is difficult to accurately understand the processes of ecosystem carbon and water cycles across different temporal and spatial scales. Large uncertainty still exists in characterizing the spatio-temporal variations of carbon and water exchanges in terrestrial ecosystems (Yuan et al., 2010; Zhang et al.,

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2010). With the advantages of systematically simulating ecosystem biogeochemical processes, terrestrial biogeochemical models, e.g., CEVSA (Cao and Woodward, 1998), BIOME-BGC (Running and Coughlan, 1988) and CENTURY (Parton et al., 1993), have been widely used as effective tools to quantify ecosystem carbon and water fluxes (Rastetter et al., 2003).

However, it is difficult or impossible to acquire all model parameters through direct measurements (Luo et al., 2001; Van Oijen et al., 2005). Uncertainties in the model predictions of carbon and water exchanges largely depend on model calibration or parameterization (Green et al., 1999; MacFarlane et al., 2000; Schulz et al., 2001; Luo et al., 2003). At observation sites, parameters can be estimated by applying model-data fusion techniques using eddy covariance and associated biometric data sets as constraints (Raupach et al., 2005; Williams et al., 2009; Wang et al., 2009). Parameter estimation with formal model-data fusion techniques refers to procedures by which the 'optimal' parameter sets giving the best agreements and model predictions (Richardson et al., 2010). Whether some model parameters can be well constrained by the data depends on the amount and quality of information in the measurements and how that information is represented in the model (Yuan et al., 2012). Initially, most analyses used only limited combination of carbon fluxes to constrain C-cycle models (e.g., Wang et al., 2001; Reichstein et al., 2003; Braswell et al., 2005; Knorr and Kattge, 2005). A number of recent studies have conclude that parameters associated with rapid relatively short timescale process such as photosynthesis are well constrained by measured CO<sub>2</sub> fluxes which contain considerable information about how "fast" processes respond to environmental drivers (Braswell et al., 2005; Friend et al., 2007; Fox et al., 2009). Parameters about "slow" processes (e.g., like the size and turnover rate of biomass, litter and soil C pools) are poorly constrained (Richardson et al., 2010; Ricciuto et al., 2011). Moreover, parameter uncertainty can be reduced as data records become longer and different types of observations are added (Richardson et al., 2010). Using multiple-constraint model data fusion technique which combines different data streams to maximize consistency among all datasets simultaneously, has become an effective procedure for estimating model parameters and model predictions (Wang and Barrett, 2003; Richardson et al., 2010; Ricciuto et al., 2011).

Here, we conducted an inverse analysis on a simplified PnET model (SIPNET) (Braswell et al., 2005) using long-term observations from three ChinaFLUX forest sites, including a temperate mixed forest, a subtropical evergreen coniferous plantation and a subtropical evergreen broad-leaved forest. We constrained the model parameters with a variety of observations, including EC measurements of net ecosystem exchanges of CO<sub>2</sub> (NEE), evapotranspiration (ET) and leaf area index (LAI) from MODIS. Our objectives were three-fold: (1) to determine the key model parameters influencing the model prediction of carbon and water fluxes; (2) to evaluate how different combinations of constraining variables influence parameter estimation and associated uncertainties; and (3) to assess the model performance with the optimized parameterization in predicting carbon and water fluxes at the three forest ecosystems.

#### 2. Materials and methods

## 2.1. Simplified Photosynthesis EvapoTranspiration (SIPNET) model

The terrestrial biogeochemical model we used in this study was the simplified Photosynthesis and EvapoTranspiration (SIP-NET) model (Braswell et al., 2005; Sacks et al., 2006), a simplified version of PnET (Aber and Federer, 1992; Aber et al., 1995, 1996). The original PnET model is simplified to decrease the number of free parameters and run time (Braswell et al., 2005; Sacks et al., 2006, 2007; Moore et al., 2008; Hu et al., 2010). SIPNET contains two vegetation carbon pools (i.e., leaves and wood carbon pools) and an aggregated soil carbon pool (Braswell et al., 2005; Sacks et al., 2006, 2007). Water flux dynamics were modeled through a sub-model of soil moisture (Sacks et al., 2006; Zobitz et al., 2008). The model performed two time steps per day: day and night. In total, the SIPNET model has 42 parameters (including initial conditions) that govern the model's behaviors (as illustrated in Appendix Table A1). The detailed description of the model has been extensively documented in Braswell et al. (2005) and Sacks et al. (2006, 2007).

In particular, as in PnET (Aber and Federer, 1992), photosynthesis in SIPNET was calculated as a maximum gross photosynthetic rate (*GPP<sub>max</sub>*) multiplied by four scalars between 0 and 1: a temperature factor ( $D_{temp}$ ), a VPD factor ( $D_{VPD}$ ), a light factor ( $D_{light}$ ) and a water factor ( $D_{water}$ ). Firstly, a potential photosynthetic rate (*GPP<sub>pot</sub>*) was calculated assuming no water stress.

$$GPP_{pot} = GPP_{max} \times D_{temp} \times D_{VPD} \times D_{light}$$
(1)

Evapotranspiration (ET) in SIPNET was consist of plant transpiration (*T*), evaporation from canopy interception ( $E_i$ ), soil evaporation ( $E_s$ ) and sublimation from the snow pack ( $S_l$ ) (if there is snow). *GPP*<sub>pot</sub>, along with the plant's water use efficiency (*WUE*) depending on vapor pressure deficit (*VPD*) was then used to calculate potential transpiration ( $T_{pot}$ ) as:

$$WUE = \frac{K_{WUE}}{VPD}$$
(2)

$$T_{pot} = \frac{GPP_{pot}}{WUE} \tag{3}$$

The total amount of water available to the plants over the course of a day  $(W_a)$  was a fraction (f) of the total amount of water in the soil (W). Actual transpiration (T) was set to the lesser of  $T_{pot}$  and  $W_a$ . Finally, GPP was computed using  $GPP_{pot}$  and  $D_{water}$ .

$$W_a = W \times f \tag{4}$$

$$\Gamma = Min(T_{pot}, W_a) \tag{5}$$

$$D_{water} = \frac{T}{T_{pot}}$$
(6)

$$GPP = GPP_{pot} \times D_{water} \tag{7}$$

#### 2.2. Study sites and data overview

Half-hourly EC flux and meteorological observations used in this study were collected from three ChinaFLUX forest sites during 2003–2008: a temperate mixed forest (CBS), a subtropical evergreen coniferous plantation (QYZ) and a subtropical evergreen broad-leaved forest (DHS). The measurements of EC flux and meteorological data at the three forest sites were made by the same instruments described by Yu et al. (2006). The characteristics of these three sites were illustrated in Table 1. More details of data collection and site description could be found in Yu et al. (2006), Zhang et al. (2006a,b), Guan et al. (2006) and Wen et al., 2006.

The ChinaFLUX data processing system described in Li et al. (2008) and Liu et al. (2012) was used to conduct quality control of the EC flux and meteorological data. After a common quality checking process (triple coordinate rotation, WPL correction, despike, absolute value and storage calculation), EC fluxes with low friction velocity ( $u^*$ ) during the night were screened out (Reichstein et al., 2005). After that, small gaps (<2 h) in EC flux records were linearly interpolated, while larger gaps were filled with the nonlinear regressions method (Liu et al., 2012). Larger gaps in meteorological records were filled using the mean diurnal variation (MDV) method (Falge et al., 2001). Climate variables at a twice-a-day time step used

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