



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 process-based 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 broad-leaved 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 growing-season 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 land-atmospheric carbon and water exchanges between terrestrial ecosystems and the atmosphere have been accumulated, mainly

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 concluded that parameters associated with rapid relatively short timescale process such as photosynthesis are well constrained by measured CO₂ 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 CO₂ (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 (SIPNET) 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_{max}) 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_{pot}) was calculated assuming no water stress.

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

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_{pot} , 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:

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

$$T_{pot} = \frac{GPP_{pot}}{WUE} \quad (3)$$

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} .

$$W_a = W \times f \quad (4)$$

$$T = \min(T_{pot}, W_a) \quad (5)$$

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

$$GPP = GPP_{pot} \times D_{water} \quad (7)$$

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

Table 1

The basic information for the three forest EC tower sites.

Site	Geographical location	Elevation (m)	Vegetation type	Observation height (m)	Annual air temperature (°C) ^a	Annual precipitation (mm) ^b	Period
CBS	41.4025° N, 128.0958° E	738	Temperate mixed forest	40	3.6	695	2003.1–2008.12
QYZ	26.7478° N, 115.0631° E	100	Subtropical evergreen coniferous plantation	39	17.9	1485	2003.1–2008.12
DHS	23.1733° N, 112.5361° E	240	Subtropical evergreen broad-leaved forest	27	20.9	1956	2003.1–2008.12

^a Mean annual air temperature of 2003–2008.^b Mean annual precipitation of 2003–2008.

for driving the SIPNET model included air temperature (T_{air} , °C), soil temperature (T_{soil} , °C), photosynthetically active radiation (PAR, $\text{mol m}^{-2} \text{ day}^{-1}$), precipitation (PRE, mm), vapor pressure deficit (VPD_{air} , Pa), vapor pressure deficit between soil and air (VPD_{soil} , Pa) and wind speed (W_s , m s^{-1}). The “daytime” and “nighttime” were defined using astronomical criteria (solar elevation greater or less than 0 °C). The half-daily NEE, gross primary productivity (GPP), ecosystem respiration (Re) and evapotranspiration (ET) were used to conduct model inversion and validation.

LAI was derived from the MODIS database for a $3 \times 3 \text{ km}^2$ area centered on each site from <http://modis.gsfc.nasa.gov/>. Additionally, to reduce the effect of cloud, the average of observation over $3 \times 3 \text{ km}^2$ areas was calculated and the 8-day composites are

linearly interpolated and smoothed with a moving average of 24 days to determine twice-a-day values.

2.3. Parameterization of SIPNET

Metropolis simulated annealing algorithms (Metropolis et al., 1953; Hurtt and Armstrong, 1996) were applied to estimate SIPNET parameters and the associated uncertainty. In general, Metropolis simulated annealing is a global optimization algorithm using a heuristic random search based on Monte Carlo's iterative solution. The optimization procedure performed a quasi-random walk through the multi-dimensional parameter space to find the parameter set that causes the model to generate the best match between

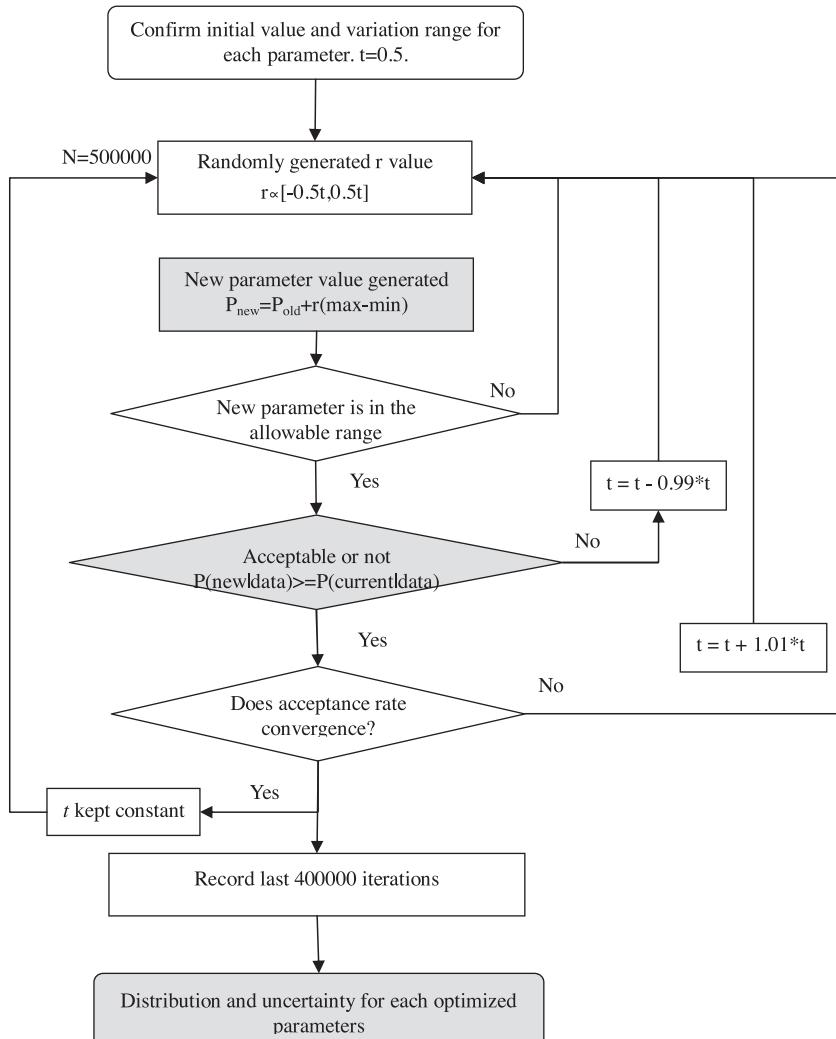
**Fig. 1.** The procedure of parameter optimization with Metropolis simulated annealing.

Table 2

The hierarchy of multi-constraint optimization experiments using the SIPNET model.

Run ID	Constraining data streams included in parameter optimization
1	NEE only all the year round
2	ET only all the year round
3	NEE and ET all the year round
4	NEE, ET and LAI all the year round
5	NEE, ET and LAI during the peak of growing season (July–August)

the predicted value and the observed value. The algorithm had three main characteristics: random walk, relaxation of acceptance criteria, and adjustment of the jump distance, which greatly improve the speed of convergence on the global optimum and limits false convergence on local optima (Zobitz et al., 2011). The specific procedures of the algorithm are as follows:

1. Confirm the initial values and variation ranges for model parameters (P) from literature-based estimates and actual measurements and then determine the value of t , which governs the fraction of the parameter's range that can be searched in a single iteration of the optimization.
2. Select a proposal parameter value generated based on t and the current value.
3. Calculate the posterior probability densities for the proposal P and the current P: $P(\text{new}|\text{data})$ and $P(\text{current}|\text{data})$. If $P(\text{new}|\text{data}) > P(\text{current}|\text{data})$, the algorithm accepts the proposal P, and decreases the value of t by a factor of 0.99. Otherwise, the proposal P is rejected and t is increased by a factor of 1.01.
4. Repeat steps 2–3 until varying any parameter leads to acceptance approximately 50% of the time. Thereafter, fix the value of t and repeat steps 2–3 for 500,000 times. The last 400,000 iterations are used to depict the posterior parameter distribution and associated uncertainty.

The detailed procedures for the Metropolis simulated annealing algorithm in this study was shown in Fig. 1, and more detailed information of the parameter estimation procedure was described by Braswell et al. (2005) and Ren et al. (2013).

To evaluate the effects of constraining variables on model optimization and prediction, we performed five optimization experiments using different constraining variables and data record length (see Table 2 for optimization experiments conducted with different data streams).

We employed leave-one-out cross validation method (Groenendijk et al., 2011; Zhang et al., 2011) to evaluate the model performance. Each of the 6 years (2003–2008) was withheld successively and then the data from the remaining 5 years were used to optimize the model parameters. The actual fluxes (i.e., NEE, GPP, RE and ET) for the omitted year was then compared to the model estimated fluxes with the optimized parameters using the training data set of all other 5 years. This procedure was repeated for each site, resulting in a number of parameters equal to the number of data years ($n = 6$ in this study). Therefore, we performed 30 optimizations for 5 experiments and 6 years at each forest ecosystem. The coefficient of determination (R^2) and root mean square error (RMSE) for comparing the measured and simulated fluxes were used to quantify the model performance.

2.4. One-at-a-time (OAT) sensitivity analysis

The One-at-a-time (OAT) approach is one of the simplest and most common sensitivity analysis methods, which repeatedly varies one parameter at a time while holding the others fixed (Gardner et al., 1980; O'Neill et al., 1980; Larocque et al., 2008). The sensitivity coefficient (β) for each parameter of SIPNET could be

Table 3

The results of the OAT sensitivity analysis for parameters of SIPNET (using QYZ as an example). Key parameters and their sensitivity coefficient (β) on the model output variables (i.e., NEE, GPP, Re, ET) at twice-a-day time step were shown.

Parameters	Ranking with β_{NEE}	β_{NEE}	β_{GPP}	β_{Re}	β_{ET}
A_d^{b}	1	1.67	1.32	0.34	0.71
A_{\max}^{b}	2	1.60	1.28	0.62	0.69
C_{frac}^{f}	3	1.60	1.28	0.63	0.69
SLW^{g}	4	1.25	0.95	0.34	0.49
k^{b}	5	0.98	0.72	0.17	0.36
$PAR_{1/2}^{\text{b}}$	6	0.94	0.60	0.14	0.27
Q_{10s}^{d}	7	0.93	0.00	0.67	0.00
Q_{10v}^{c}	8	0.78	0.09	0.37	0.05
T_{opt}^{b}	9	0.55	0.36	0.42	0.13
A_L^{f}	10	0.54	0.33	0.32	0.20
K_F^{b}	11	0.48	0.04	0.37	0.02
K_I^{f}	12	0.43	0.31	0.25	0.18
K_{WUE}^{e}	13	0.42	0.23	0.09	0.49
LAI^{a}	14	0.33	0.24	0.17	0.15
W_S^{e}	15	0.32	0.17	0.06	0.23
R_{sc1}^{e}	16	0.23	0.14	0.06	1.02
T_{min}^{b}	17	0.17	0.10	0.02	0.03
f^{e}	18	0.06	0.03	0.01	0.12
R_{sc2}^{e}	19	0.05	0.03	0.01	0.24
R_d^{e}	20	0.03	0.02	0.01	0.37

^a Initial state values.

^b Photosynthesis parameters.

^c Autotrophic respiration parameters.

^d Soil respiration parameters.

^e Moisture parameters.

^f Tree physiological parameters.

determined by calculating the variation percentage of each model output variables due to the 1% variation of each parameter (Eq. (8)).

$$\beta = \frac{VR}{\Delta P} \quad (8)$$

where VR was the variation percentage (%) of model output variables when ΔP varies for the parameter (or variable) P. In this study, each parameter of the SIPNET model was varied by $\pm 10\%$ (i.e., $\Delta P = 20\%$), and VR is calculated as follows:

$$VR = 100 \times \frac{|run_{+10\%} - run_{-10\%}|}{run_{ref}} \quad (9)$$

where $run_{+10\%}$ and $run_{-10\%}$ were the predictions with +10% and -10% variations in a given parameter (or variable) and other parameters and variables are fixed; run_{ref} were the predictions of reference simulations with all parameters or variables unchanged.

In this study, NEE, GPP, RE and ET at twice-a-day time step during 2003–2008 were selected as the main model output variables. The mean value of sensitivity coefficient (β) for model output variables at twice-a-day time step was calculated to represent of the ratio of the change in the model output variables to the change in the model parameter. Then the effects of all parameters on each model output variable can be ranked from the averaged β .

3. Results

3.1. Key model parameters for model prediction

With the OAT sensitivity analysis, the parameters had significant influence of the output variables of SIPNET was similar across three forest ecosystems, with slight difference in the sensitivity ranking. Among the 42 model parameters (Table A1), 20 parameters with a averaged sensitivity coefficient great than 0.1 on NEE, GPP, Re or ET (i.e. the variation percentage of model output due to the 1% variation of each parameter $> 0.1\%$) have been considered as key model parameters (Table 3 using QYZ as an example; full description of the parameters were shown in Table A1). The key parameters could be classified into five types:

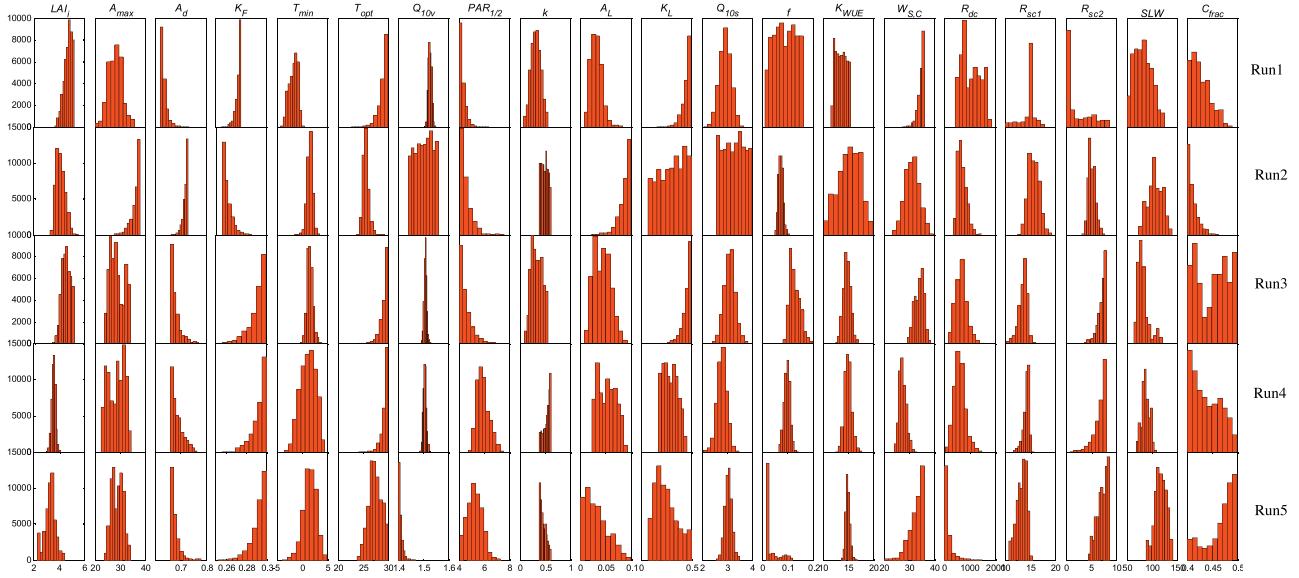


Fig. 2. The posterior distribution of parameters deduced from five experiments as listed in Table 2 (using CBS in 2006 as an example). The X axis represents the parameters' value, while the Y axis represents the frequency.

1. *Initial state values*: initial leaf area index (LAI_i).
2. *Photosynthesis-related parameters*: average daily maximum photosynthesis as fraction of A_{max} (A_d), maximum net CO₂ assimilation rate (A_{max}), canopy PAR extinction coefficient (k), half saturation point of PAR-photosynthesis relationship ($PAR_{1/2}$), optimum temperature for photosynthesis (T_{opt}), foliar maintenance respiration as fraction of A_{max} (K_F), and minimum temperature for photosynthesis (T_{min}).
3. *Respiration-related parameters*: soil respiration Q_{10} (Q_{10s}), and vegetation respiration Q_{10} (Q_{10v}).
4. *Moisture parameters*: VPD-water use efficiency relationship (K_{WUE}), soil water holding capacity (W_{sc}), scalar relating soil resistance to soil wetness (R_{sc1}, R_{sc2}), fraction of soil water removable in one day (f), and scalar relating aerodynamic resistance to wind speed (R_d).
5. *Tree physiological parameters*: fractional carbon content of leaves (C_{frac}), carbon content of leaves on a per-area basis (SLW), fraction of mean NPP allocated to leaf growth (A_L), and turnover rate of leaf carbon (K_L).

For NEE, four parameters, including two photosynthesis-related parameters (A_d and A_{max}) and two tree physiological parameter (C_{frac} and SLW), had significant effects on the modeled NEE with a β value greater than 1.0. Meanwhile, A_d , A_{max} and C_{frac} were also the most three sensitive parameters influencing GPP predication and Q_{10s} has the strongest effect on modeled Re. The similar sorting order of parameter on GPP and NEE, indicating that photosynthesis was the dominant process of the ecosystem's carbon cycle. The modeled ET was most sensitive to R_{sc1} . Besides, ET and GPP almost had the same top 5 key parameters, including A_d , A_{max} , C_{frac} and SLW , reflecting the coupling between ecosystem carbon and water flux dynamics.

3.2. The constraining effect of variables on model parameters

Observations of NEE, ET or LAI illustrated in five optimization experiments (Table 2) were used to constrain the SIPNET parameters. We estimated the posterior PDFs of 20 key parameters using Metropolis simulated annealing algorithms. Depending upon the shape of posterior distributions (Fig. 2, with CBS in 2006 as an example), the optimized parameters could be classified into

three groups: well-constrained, poorly constrained and edge hitting, which could demonstrate the constraining effect of variables on model parameters and predictions.

The parameters were thought to be well-constrained by the measurements if their posterior distributions approximated to normal distribution (Braswell et al., 2005). Our analyses indicated that seven key parameters could be well constrained by NEE, which mainly included the photosynthesis-related parameters (A_{max} , k and T_{min}), respiration-related parameters (Q_{10s} and Q_{10v}), and tree physiological parameters (A_L and SLW). Six moisture parameters (i.e., K_{WUE} , f , W_{sc} , R_d , R_{sc1} , and R_{sc2}) could be well constrained by ET. When both year-round NEE and ET were used in optimizing model parameters, 11 parameters could be well constrained. Moreover, when LAI was added, two more parameters related to initial state values (LAI_i) and photosynthesis ($PAR_{1/2}$) could be well-constrained. For NEE and ET during the peak of growing season, only six parameters could be well-constrained.

The posterior distributions of those parameters with edge hitting patterns were often concentrated on the values in proximity to the extreme values of the parameters' ranges. In the optimization with year-round NEE as constrained variables (Run 1), seven parameters (e.g., A_d and K_F) had a skewed distribution. With year-round ET as the constraining variables (Run 2), the posterior distribution of six parameters (e.g., A_{max} and A_L) were edge hitting. When NEE and ET were used together in parameter optimization (Run 3), six parameters were also edge hitting. The edge hitting may be partly due to the insignificant constraining role of the data in the model's parameters and the limit of model's parameter threshold (Braswell et al., 2005).

The posterior distributions of the poorly constrained parameters were uniformly distributed. Except one moisture parameter (i.e., f) in the carbon-only optimization experiment (Run 1), and three parameters related to respiration and tree physiology (Q_{10v} , Q_{10s} and K_L) in the water-only optimization (Run 2) were uniformly distributed, few poorly constrained parameters were found in the other three optimization experiments.

Overall, NEE observations had significant roles in constraining 19 out of 20 model parameters. When only ET was used to constrain the model's parameters, some parameters in the model, particularly the respiration-related ones, were poorly constrained with uniform posterior distributions. When LAI was added to the

Table 4

Average and standard deviations (in brackets) of the SIPNET parameters at three forest ecosystems during 2003–2008.

Parameters	CBS	QYZ	DHS
A_d	0.73 (0.08)	0.76 (0.09)	0.75 (0.06)
A_{max}	25.98 (4.73)	24.05 (5.74)	23.12 (1.98)
C_{frac}	0.46 (0.02)	0.46 (0.03)	0.45 (0.03)
SLW	93.87 (19.88)	65.72 (5.69)	63.94 (2.45)
k	0.56 (0.05)	0.54 (0.08)	0.53 (0.05)
$PAR_{1/2}$	4.03 (0.02)	4.53 (0.43)	4.66 (0.27)
Q_{10s}	2.54 (0.32)	1.69 (0.13)	1.71 (0.07)
Q_{10v}	1.47 (0.05)	1.68 (0.13)	1.8 (0.17)
T_{opt}	29.98 (0.01)	29.98 (0.04)	29.96 (0.04)
A_L	0.36 (0.08)	0.15 (0.23)	0.3 (0.02)
K_F	0.29 (0.01)	0.11 (0.05)	0.06 (0.01)
K_L	0.5 (0.01)	0.15 (0.17)	0.93 (0)
K_{WUE}	14.93 (0.78)	13.99 (0.21)	9.53 (0.14)
LAI_i	3.81 (0.27)	4.23 (0.62)	3.65 (0.25)
W_c	17.41 (5.14)	24.67 (1.51)	28.38 (1.15)
R_{sc1}	11.75 (2.22)	9.76 (1.58)	14.6 (0.66)
T_{min}	4.24 (0.25)	-5.67 (1.03)	-6.6 (1.29)
f	0.04 (0.02)	0.12 (0.05)	0.03 (0)
R_{sc2}	6.39 (2.49)	4.13 (1.6)	8.1 (0.67)
R_d	238.19 (99.17)	113.14 (85.26)	3.06 (1.47)

optimization (Run 4), the number of well-constrained parameters was increased. In particular, when the model was constrained with ET and NEE during the peak of growing season, the posterior distribution of the model's parameters change from normal distribution to skewed distribution, suggesting the sample size and temporal representativeness of the constraining variables had important impacts on the estimation of model parameters.

3.3. Optimized parameters and associated uncertainty

From the results of the optimized parameters, it could be observed that the posterior distributions of some parameters were not normal (see Fig. 2). The posterior mean value and standard deviation could not fully describe the parameter posterior distribution. Therefore, the 'optimal' estimation and confidence interval must be used to describe the distribution. The posterior statistics of optimized parameters under five experiments were shown in Fig. 3 ('optimal' estimates and 90% confidence interval for optimized parameters in CBS in 2006 are taken as an example). When only NEE was used to constrain the model's parameters (Run 1), it lead to significant uncertainty of the results, although its constraining effect was better than ET alone (Run 2). Including the NEE and ET data simultaneously (Run 3) tends to result in narrower confidence intervals compared to when only NEE or ET data were used (Runs 1 and Run 2). Compared to the tower NEE and ET measurements, we also found that LAI measurements, to a lesser degree, contributed reductions in uncertainties in parameter estimates. Furthermore, instead of involving the year-round observations in constraining the model's parameters, using only the data in the growing peak season (Run 5) significantly increased the uncertainty of estimated parameters.

Although different optimization experiments in the same ecosystem may lead to different 'optimal' estimates and confidence intervals of the model parameter, these differences were not large enough to affect the parameter comparison among different forest ecosystems (Table 4). Overall, the differences in the results of the optimized parameters for the three different forest ecosystems depend on specific parameters. Among the three forest ecosystems, several parameters show great difference from each other. Specifically, A_{max} in CBS (25.98 nmol CO₂ g⁻¹ s⁻¹) is significantly higher than that in QYZ (24.05 nmol CO₂ g⁻¹ s⁻¹) and DHS (23.12 nmol CO₂ g⁻¹ s⁻¹). This was also the case for the SLW, Q_{10s} , R_{sc1} , R_{sc2} and W_c in CBS compared with those in QYZ and DHS. For K_{WUE} and R_d ,

Table 5

The model performance (i.e., coefficient of determination – R^2 and root mean square error – RMSE) for the five experiments illustrated in Table 2 in three forest ecosystems in China.

Fluxes	Run ID	CBS		QYZ		DHS	
		R^2	RMSE	R^2	RMSE	R^2	RMSE
NEE	1	0.84	1.01	0.91	0.90	0.91	0.63
	2	0.57	7.94	0.43	6.61	0.53	6.55
	3	0.83	1.06	0.92	0.83	0.91	0.64
	4	0.82	1.07	0.87	1.05	0.90	0.66
	5	0.82	1.18	0.86	1.06	0.82	1.02
ET	1	0.25	0.08	0.41	0.09	0.10	0.12
	2	0.81	0.04	0.78	0.06	0.80	0.04
	3	0.74	0.05	0.77	0.06	0.78	0.05
	4	0.74	0.05	0.82	0.05	0.80	0.05
	5	0.71	0.05	0.48	0.10	0.72	0.05

the optimal value in CBS was the greatest, which were followed by QYZ and DHS.

3.4. Overall agreement between observation and model predictions with optimized parameters

With the 'optimal' parameters in three forest ecosystems, simulation performances of SIPNET for five experiments (Table 2) were illustrated using a Taylor Diagram (Fig. 4), which could intuitively demonstrate the consistency between the simulated values and measured data. According to the mathematical meaning of the Taylor Diagram (Taylor, 2001), four statistical quantities are geometrically connected: the correlation coefficient (r), the standard deviation (SD) of observation, the SD of model simulation, and the centered pattern root-mean-square. The polar axis displays the correlation coefficient and the radial axes display the root mean standard deviation (RMSD) of the modeled variable. The *Obs* point in the figure means the simulated value is the same as the measured value and the correlation coefficient is 1. Simulated values in agreement with the observed values will lie near the *Obs* point, with relatively high r and low RMSD.

The assessment of model performance indicated that carbon and water exchanges could be well simulated by the SIPNET model with 'optimal' parameters in Run 3 for three forest ecosystems in China (Fig. 4). However, if only using the ET (or NEE) data to constrain the model and simulate the ecosystem's NEE (or ET), there will be great difference between the model predictions and observations. This indicated that although there was a strong coupling between the ecosystem carbon and water exchange processes, only using a certain type of data to constrain the model and predict the ecosystem's overall carbon and water exchanges could result in great deviation. Including year-round LAI to the optimization (Run 4), the model performance was basically conform to the result in experiment 3, with the model fit to the observed NEE fluxes reduced and to the observed ET increased only slightly. As for the measured data with different data record length, the consistency between simulated and measured values of NEE and ET using only the measured data in the peak growing seasons was lower than that in Run 3 and Run 4. This finding suggested that careful consideration should be given to the temporal representativeness of constraining data when optimizing the model's parameters for ecosystems with distinct seasonal variations.

Specifically, in the process of extrapolating the 'optimal' parameter set acquired with leave-one-out cross method using both year-round NEE and ET as model constraints (Run 3), the mean value R^2 of simulated NEE for CBS, QYZ and DHS during the study period were calculated to be 0.83, 0.92 and 0.91, respectively (Table 5). The simulation performances for ET were generally lower than that for NEE ($R^2 = 0.74$, 0.77 and 0.78 for three forest

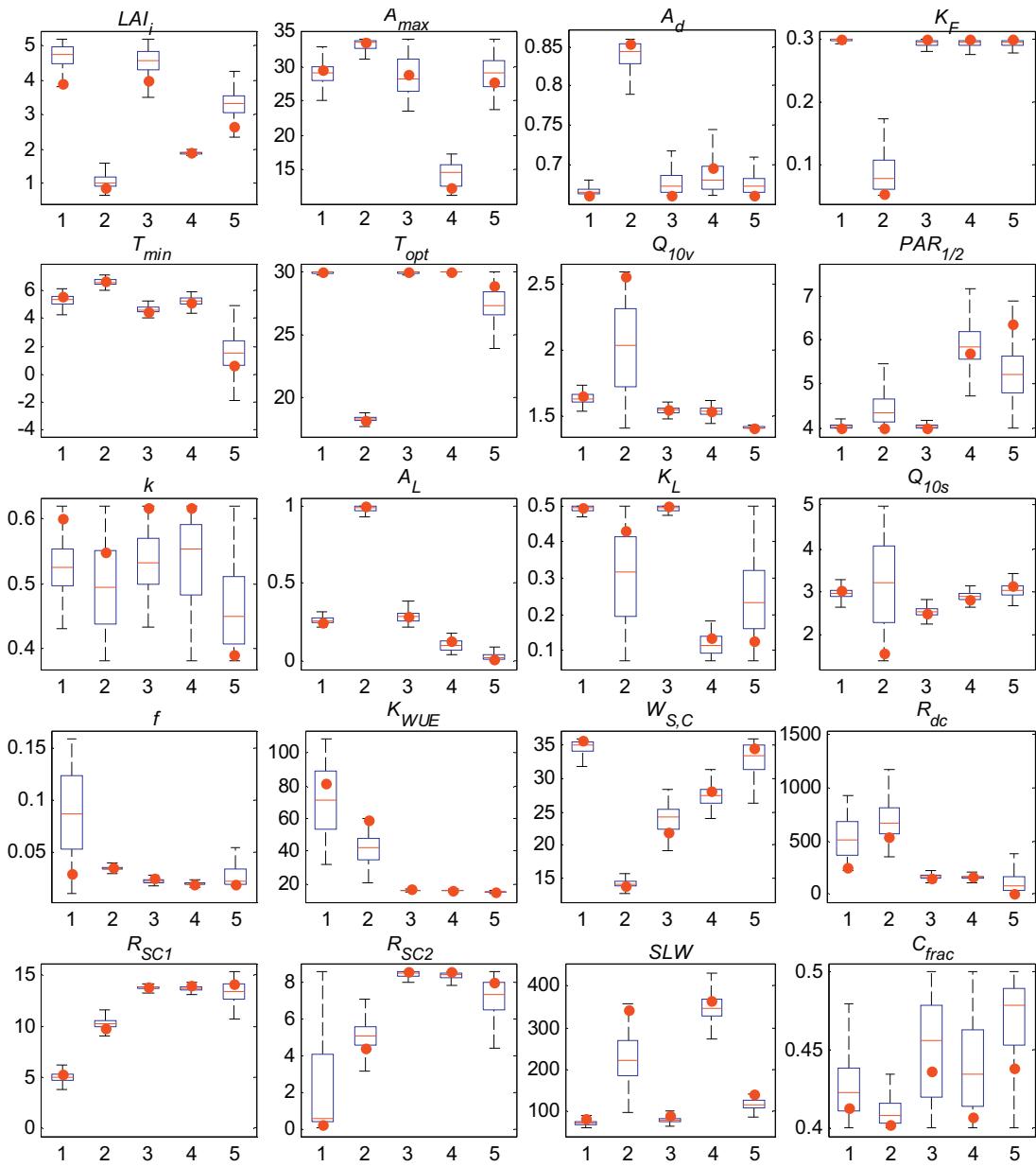


Fig. 3. A box diagram of parameters estimated for SIPNET using different data constraints (using CBS in 2006 as an example). The X axis represents the number of five experiments as illustrated in Table 2, while the Y axis represents the simulated values of the parameters. The red solid dot is the 'optimum' estimates of the parameter set. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

ecosystems, respectively). Overall, using the 'optimal' value of optimized parameters based on year-round NEE and ET could simulate the carbon and water fluxes in three forest ecosystems in China (Fig. 5).

4. Discussion

We have used a variety of different variables from EC observations (i.e., NEE and ET) and MODIS products (LAI) to constrain the key parameters of the SIPNET model for three forest ecosystems in China. In our study, OAT sensitivity analysis, a local sensitivity analysis method, was performed to rank key parameters of SIPNET by calculating the ratio of model results while the input parameter was varied by $\pm 10\%$. The sensitivity results showed that, among three different forest ecosystems, the prediction of NEE, GPP, Re and ET were mostly affected by photosynthesis-related parameters. Although

OAT sensitivity analysis was a local approach, it reached the similar rankings of the top several sensitive parameters of ecosystem processed models with global sensitivity analysis approaches (Tang and Zhuang, 2009; Yu and Harris, 2009). For example, using a global sensitivity analysis with the first-order impact ratio (FOIR), Tang and Zhuang (2009) found that the simulated carbon fluxes of terrestrial ecosystem model (TEM) were mostly affected by three photosynthesis-related parameters (i.e., the maximum rate of photosynthesis, the half-saturation constant for CO₂ uptake by plants, and the half-saturation constant for photosynthetically active radiation used by plants). Using fourteen methods of parameter sensitivity analysis, Hamby (1995) pointed out that both local and global techniques resulted in similar rankings of the top several sensitive parameters. The simplest among the sensitivity analysis methods used produced results comparable to those obtained by methods more computationally expensive (Confalonieri et al., 2010). Theoretically, the

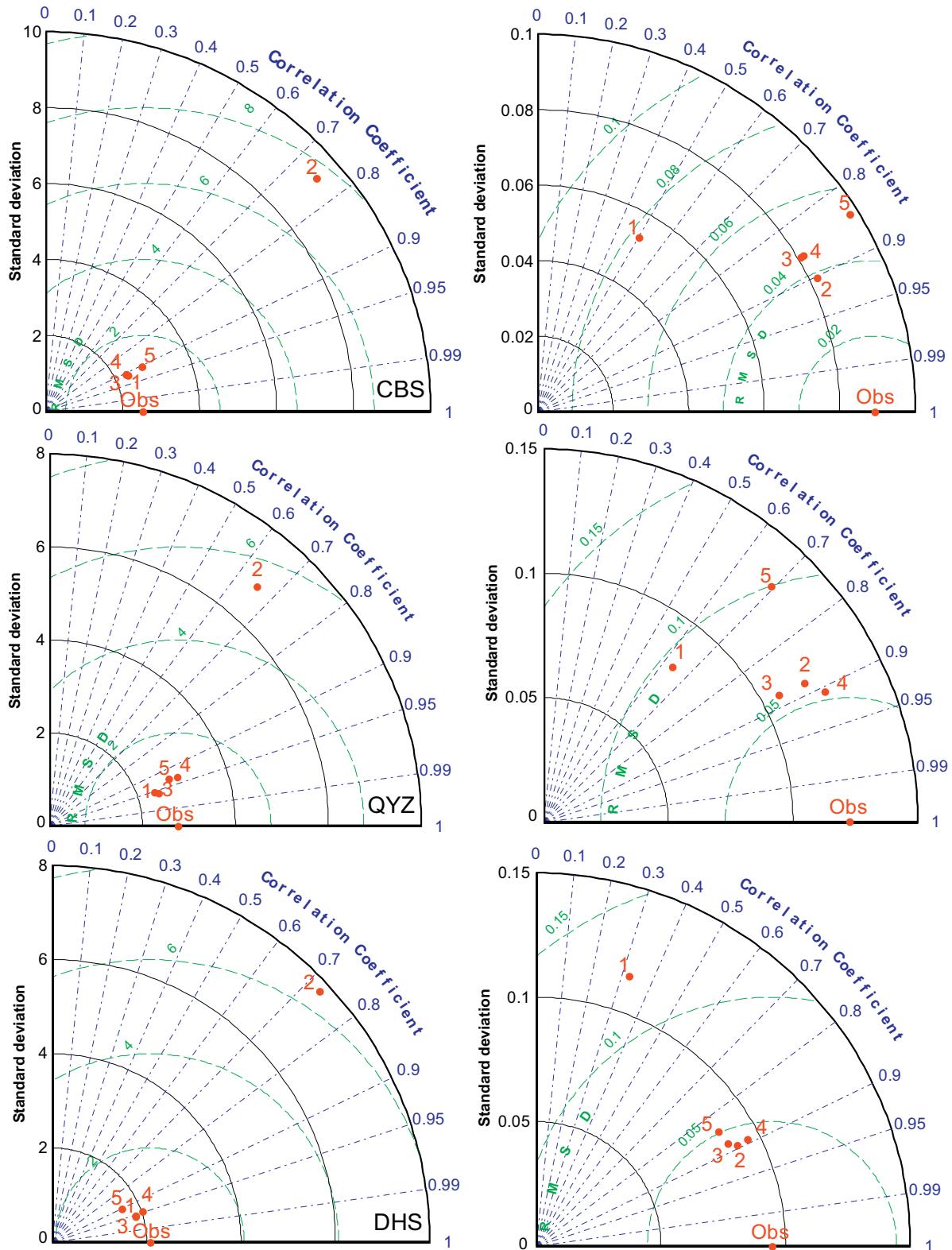


Fig. 4. The Taylor Diagram for the simulation performance of SIPNET in three forest ecosystems. The values in the diagram are calculated on the basis of the observations (i.e., NEE and ET), as well as the model simulation during 2003–2008. The red numbers (i.e., 1–5) depict the five experiments illustrated in Table 2. The three diagrams on the left are the results for NEE, while the three on the right are for ET. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

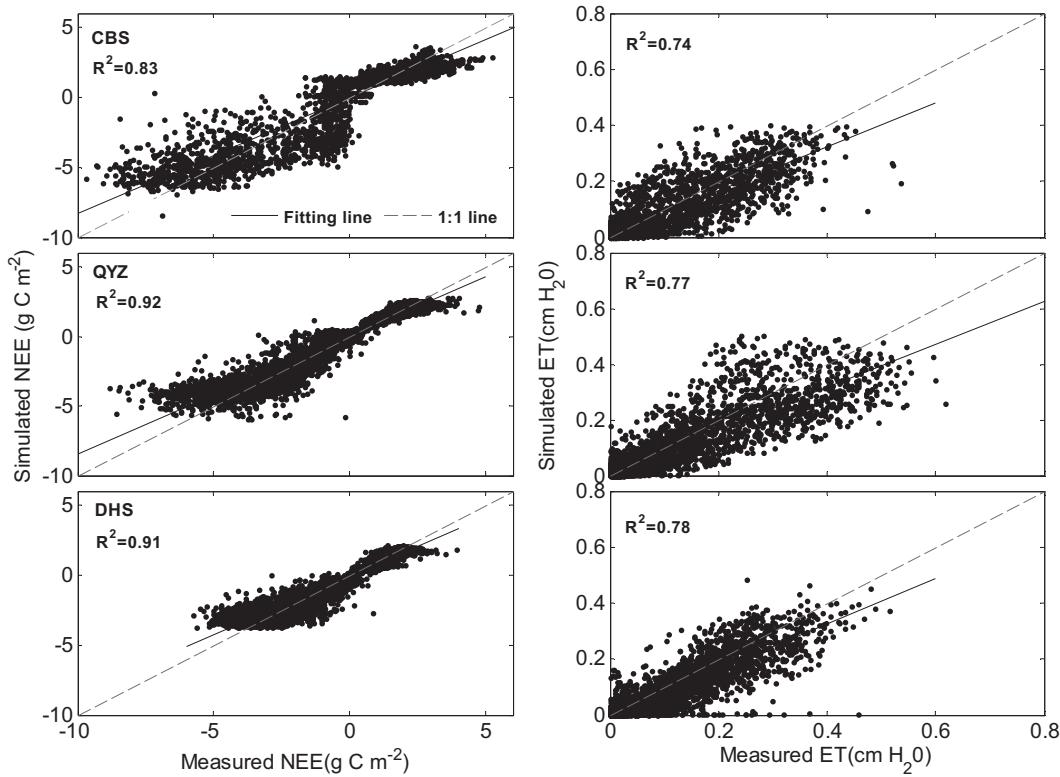


Fig. 5. Comparison between the simulated and measured values of NEE and ET for 2003–2008, using the SIPNET parameterized with leave-one-out cross method using NEE and ET as model constraints. The dotted gray lines represent the 1:1 lines, and the black solid lines represent the linear fitting relationships.

dominant influence of photosynthesis parameters on the simulation of carbon fluxes of process-based biogeochemistry models maybe due to the fact that GPP was a major determination of carbon and water exchange between terrestrial ecosystems and atmosphere (Richardson et al., 2010). The appropriate method to identify the model key parameters will depend on the research question being addressed.

Previous studies have reported limited success in estimating model parameters using eddy flux alone. For example, Wang et al. (2001, 2007) and Knorr and Kattge (2005) found that only 3–6 parameters could be well-constrained. Here, in the first experiment, using NEE observations only (Run 1), posterior distributions were poorly constrained for most moisture parameters; there were large errors in ecosystem ET simulations when compared with observations from these unreasonable parameters values (Fig. 4). Similarly, the study by Moore et al. (2008) showed that the carbon-only optimization was insensitive to imposed changes in water availability. The lack of constraint by observed ET allowed the model to move water-use efficiency to unrealistically high values during the parameterization process (Fig. 5). In ET-only mode (Run 2), as showed in the second experiment, the respiration-related parameters were poorly constrained with uniform posterior distributions, which lead the most deviation between observation and simulation of NEE (Fig. 5). In Run 1 and Run 2, the poorly constrained parameters made the simulated results deviate significantly from their measured values. We observed that in the carbon-only experiment, the lack of constraint by observed ET resulted in a dramatically underestimate of the magnitude of T , which moved the linkage between GPP and T , expressed as water use efficiency, to unrealistically high values. This could be due to the model attempt to increase E_s to balance seasonal dynamics in the soil moisture content. Similar results were also occurred in the water-only experiment. These two experiments indicated

that although there was a strong coupling between the ecosystem carbon and water exchange processes, and the inter-relationship linkage was also simulated in the model, only using a certain type of data to constrain the model could result in great deviation. In contrast, the coupled NEE/ET optimization in the third experiment resulted well-constrained parameters and a far more plausible simulation of both NEE and ET. Beyond the tower fluxes, while LAI were used simultaneously as joint constraints, the number of well-constrained model parameters was increased. However, compared the experiment with NEE and ET as constraints, the model performance in experiment four with LAI added were not improved significantly. We expected this minimal contribution of canopy structural data was related to the relationship between LAI and GPP. Because GPP was a major determinant of NEE, there was already information on LAI contained in the NEE time series.

With year-round NEE and ET as model constraints, in the third model experiment, it showed there were great variations in the magnitude of ecosystem A_{max} and K_{WUE} . The ecosystem A_{max} at CBS was higher than that of QYZ and DHS, while both QYZ and DHS were evergreen forest (Table 1). The probable reasons might be related to the limited growing season at CBS. Studies have demonstrated that the photosynthetic capacity of forest ecosystems with limited growing season usually was higher than forests that carried multiple years of foliage (Falge et al., 2002; Zhang et al., 2006a,b). A representation of the carbon-water coupling in the model could only be achieved when the model was informed by observation of the carbon and water fluxes (Moore et al., 2008). K_{WUE} , the relationship between the plant's photosynthesis without water stress (GPP_{pot}) and plant's potential transpiration (T_{pot}), was a key indicator in SIPNET to fully understand the coupling between carbon and water cycles within ecosystems. The high K_{WUE} by the optimization indicated that there was less water stress at the site, which

was proved in three forest ecosystems of this study. According to actual GPP and ET at twice-day step, there exists a stronger linear linkage between water and carbon fluxes in CBS, whereas the linkage between GPP and ET in DHS and QYZ showed quadratic curves. It was partly caused by the severe drought on QYZ and excessive rainfall at DHS, which were not favor to ecosystem photosynthesis.

Our current analysis also extended our understanding of how to design effective model-data fusion scheme given specific aims in the use of a model. It was sufficient with SIPNET to only constrain parameter estimation using NEE when we only interested in using the model to inform us about NEE and its components. The NEE-only experiment contained no insight with which to inform the relative magnitudes of components of ET. However, even with LAI data streams as constraints, we were not able to derive all the key parameters successfully. Other inverse analyses have reached the same conclusions (e.g., Braswell et al., 2005; Richardson et al., 2010). In order to increase the number of constrained parameters, many studies have been conducted with increasing data used (Moore et al., 2008; Richardson et al., 2010), altering model structures (Chatfield, 1995), improving optimization methods (Wu et al., 2009) and considering the internal relationship among ecosystem processes (Yuan et al., 2012). In this study, we were aimed to improve the performances of the model simulations on NEE and ET, the parameterization scheme using both net ecosystem exchange (NEE) and evapotranspiration (ET) as constraining variables performed best with most well-constrained parameters. In the experiment, a plausible representation of the carbon–water coupling could be achieved when the model was informed by the observations of carbon and water fluxes. Increasing data streams in constraining model parameters does not necessarily make for a better performance.

5. Conclusions

Measurements from eddy covariance sites provide rich source of information for evaluating model representations of CO₂ and H₂O exchange with the atmosphere. Using the eddy covariance flux measurement and leaf area index (LAI) from MODIS at three forest ecosystems, this modeling study demonstrated that the photosynthesis-related parameters have significant impacts on the SIPNET model simulation. We found that when NEE and ET were jointly used to constrain the model, the number of well-constrained model parameters increases, leading to improvement of the model simulation accuracy. 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. Meanwhile, optimized parameters and associated uncertainties were largely influenced by the sample size and time representativeness of the observation data, especially for the ecosystem with distinct seasonal variations.

Our analysis has shown that there is a role for model-data fusion analyses in studies connecting the carbon and water cycles in forested ecosystems. Given that several flux observations sites were achieved continuous measurements, there was tremendous potential in the use of ecosystem process models to conduct comparative analysis on those parameters that most control patterns of carbon sequestration and water loss.

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Appendix A.

See Table A1.

Table A1

The description of the SIPNET model parameters, including initial conditions.

Parameter symbol	Definition	Units
<i>Initial state values</i>		
$C_{w,0}$	Initial plant wood carbon content	g C m ⁻² (ground)
<i>Photosynthesis parameters</i>		
A_{max}	Maximum net CO ₂ assimilation rate	nmol CO ₂ g ⁻¹ (leaf) s ⁻¹
A_d	Average daily maximum photosynthesis as fraction of A_{max}	–
K_F	Foliar maintenance respiration as fraction of A_{max}	–
T_{min}	Minimum temperature for photosynthesis	°C
T_{opt}	Optimum temperature for photosynthesis	°C
K_{VPD}	Slope of VPD-photosynthesis relationship ($D_{VPD} = 1 - K_{VPD} \cdot VPD^{E_{VPD}}$)	kPa ⁻¹
E_{VPD}	Exponential of VPD-photosynthesis relationship ($D_{VPD} = 1 - K_{VPD} \cdot VPD^{E_{VPD}}$)	–
$PAR_{1/2}$	Half saturation point of PAR-photosynthesis relationship	mol m ⁻² (ground) day ⁻¹
k	Canopy PAR extinction coefficient	–
<i>Phenology parameters</i>		
D_{on}	Day of year for leaf out	Day of year (DOY)
GDD_{on}	Growing degree days (GDD) threshold for leaf appearance	°C day
T_{on}	Soil temperature threshold for leaf appearance	°C
D_{off}	Day of year for leaf drop	Day of year (DOY)
L_g	Leaf growth at start of growing season	g C m ⁻² (ground)
L_f	Fraction of leaves that fall at end of growing season	–
<i>Autotrophic respiration parameters</i>		
K_A	Wood respiration rate at 0 °C	g C g ⁻¹ C year ⁻¹
Q_{10v}	Vegetation respiration Q_{10}	–
S_{fa}	Amount that foliar respiration is shutdown if soil is frozen	–
S_{ft}	Threshold of soil temperature below which S_{fa} and f_f kick in	°C
<i>Soil respiration parameters</i>		
K_s	Soil respiration rate at 0 °C and moisture-saturated soil	g C g ⁻¹ C year ⁻¹

Table A1 (Continued)

Parameter symbol	Definition	Units	Seasonality of ecosystem respiration and gross primary production as derived from FLUXNET measurements. <i>Agric. For. Meteorol.</i> 113, 53–74.
$Q_{10,S}$	Soil respiration Q_{10}	–	Fox, A., Williams, M., Richardson, A.D., Cameron, D., Gove, J.H., Quaife, T., Ricciuto, D., Reichstein, M., Tomelleri, E., Trudinger, C.M., Van Wijk, M.T., 2009. The REFLEX project: comparing different algorithms and implementations for the inversion of a terrestrial ecosystem model against eddy covariance data. <i>Agric. For. Meteorol.</i> 149, 1597–1615.
R_{sm}	Scalar determining the effect of soil moisture on soil respiration	–	Friend, A.D., Arneth, A., Kiang, N.Y., Lomas, M., Ogee, J., Rodenbeck, C., Running, S.W., Santaren, J.D., Sitch, S., Viovy, N., Woodward, F.I., Zaehle, S., 2007. FLUXNET and modelling the global carbon cycle. <i>Glob. Change Biol.</i> 13, 610–633.
<i>Moisture parameters</i>		Gardner, R.H., Huff, D.D., O'Neill, R.V., Mankin, J.B., Carney, J., Jones, J., 1980. Application of error analysis to a marsh hydrology model. <i>Water Resour. Res.</i> 16, 659–664.	
E	Fraction of rain immediately intercepted and evaporated	–	Green, E.J., MacFarlane, D.W., Valentine, H.T., Strawderman, W.E., 1999. Assessing uncertainty in a stand growth model by Bayesian synthesis. <i>For. Sci.</i> 45, 528–538.
f_d	Fraction of water entering soil that goes directly to drainage	–	Groenendijk, M., Dolman, A.J., Ammann, C., Arneth, A., Cescatti, A., Dragoni, D., Gash, J.H.C., Guelisse, D., Gioli, B., Kiely, G., Knol, A., Law, B.E., Lund, M., Marcolla, B., van den Molen, M.K., Montagnani, L., Moors, E., Richardson, A.D., Roupsard, O., Verbeeck, H., Wohlfahrt, G., 2011. Seasonal variation of photosynthetic model parameters and leaf area index from global Fluxnet eddy covariance data. <i>J. Geophys. Res. Biogeosci.</i> , 116.
V_s	Snow melt rate	cm H ₂ O equiv °C ⁻¹ day ⁻¹	Guan, D.X., Wu, J.B., Zhao, X.S., Han, S.J., Yu, G.R., Sun, X.M., Jin, C.J., 2006. CO ₂ fluxes over an old, temperate mixed forest in northeastern China. <i>Agric. For. Meteorol.</i> 137, 138–149.
f	Fraction of soil water removable in 1 day	–	Hamby, D.M., 1995. A comparison of sensitivity analysis techniques. <i>Health Phys.</i> 68, 195–204.
f_f	Fraction of soil water that's available if soil is frozen	–	Hu, J., Moore, D.J.P., Burns, S.P., Monson, R.K., 2010. Longer growing seasons lead to less carbon sequestration by a subalpine forest. <i>Glob. Change Biol.</i> 16, 771–783.
K_{WUE}	VPD-water use efficiency relationship	mg CO ₂ kPa g ⁻¹ H ₂ O	Hurtt, G.C., Armstrong, R.A., 1996. A pelagic ecosystem model calibrated with BATS data. <i>Deep Sea Res. Part II Topical Stud. Oceanogr.</i> 43, 653–683.
$W_{S,C}$	Soil water holding capacity	cm (precip equiv)	Knorr, W., Katte, J., 2005. Inversion of terrestrial ecosystem model parameter values against eddy covariance measurements by Monte Carlo sampling. <i>Glob. Change Biol.</i> 11, 1333–1351.
R_d	Scalar relating aerodynamic resistance to wind speed ($r_d = R_d/u$)	–	Larocque, G.R., Bhatti, J.S., Liu, J.X., Ascough, J.C., Luckai, N., Gordon, A.M., 2008. The importance of uncertainty and sensitivity analyses in process-based models of carbon and nitrogen cycling in terrestrial ecosystems with particular emphasis on forest ecosystems. Selected papers from a workshop organized by the International Society for Ecological Modelling (ISEM) at the third biennial meeting of the International Environmental Modelling and Software Society (IEMSS) in Burlington, Vermont, USA, August 9–13, 2006 Preface. <i>Ecol. Model.</i> 219, 261–263.
R_{SC1}	Scalar relating soil resistance to soil wetness ($r_{soil} = e^{R_{soil,1}-R_{soil,2}(W/W_c)}$)	–	Li, C., He, H., Liu, M., Su, W., Fu, Y., Zhang, L., Wen, X., Yu, G., 2008. The design and application of CO ₂ flux data processing system at ChinaFLUX. <i>J. Geoinf. Sci.</i> 10, 557–565 (in Chinese with English abstract).
R_{SC2}	Scalar relating soil resistance to soil wetness ($r_{soil} = e^{R_{soil,1}-R_{soil,2}(W/W_c)}$)	–	Liu, M., He, H.L., Yu, G.R., Sun, X.M., Zhang, L., Han, S.J., Wang, H.M., Zhou, G.Y., 2012. Uncertainty analysis in data processing on the estimation of net carbon exchanges at different forest ecosystems in China. <i>J. For. Res.</i> 17, 312–322.
<i>Tree physiological parameters</i>		Luo, Y.Q., Wu, L.H., Andrews, J.A., White, L., Matamala, R., Schafer, K.V.R., Schlesinger, W.H., 2001. Elevated CO ₂ differentiates ecosystem carbon processes: deconvolution analysis of Duke Forest FACE data. <i>Ecol. Monogr.</i> 71, 357–376.	
SLW	Carbon content of leaves on a per-area basis	g C m ⁻² (leaf)	Luo, Y.Q., White, L.W., Canadell, J.G., DeLucia, E.H., Ellsworth, D.S., Finzi, A.C., Lichter, J., Schlesinger, W.H., 2003. Sustainability of terrestrial carbon sequestration: a case study in Duke forest with inversion approach. <i>Glob. Biogeochem. Cycles</i> 17, 1021, http://dx.doi.org/10.1029/2002GB001923 .
C_{frac}	Fractional carbon content of leaves	g C g ⁻¹ (leaf)	MacFarlane, D.W., Green, E.J., Valentine, H.T., 2000. Incorporating uncertainty into the parameters of a forest process model. <i>Ecol. Model.</i> 134, 27–40.
A_L	Fraction of mean NPP allocated to leaf growth	–	Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N., Teller, A.H., Teller, E., 1953. Equation of state calculations by fast computing machines. <i>J. Chem. Phys.</i> 21, 1087–1092.
K_L	Turnover rate of leaf carbon	g C g ⁻¹ C year ⁻¹	Moore, D.J.P., Hu, J., Sacks, W.J., Schimel, D.S., Monson, R.K., 2008. Estimating transpiration and the sensitivity of carbon uptake to water availability in a subalpine forest using a simple ecosystem process model informed by measured net CO ₂ and H ₂ O fluxes. <i>Agric. For. Meteorol.</i> 148, 1467–1477.
K_w	Turnover rate of plant wood carbon	g C g ⁻¹ C year ⁻¹	O'Neill, R.V., Gardner, R.H., Mankin, J.B., 1980. Analysis of parameter error in a non-linear model. <i>Ecol. Model.</i> 8, 297–311.

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