

# Uncertainty analysis in data processing on the estimation of net carbon exchanges at different forest ecosystems in China

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**Abstract** Information about the uncertainties associated with eddy covariance observations of surface-atmosphere CO<sub>2</sub> exchange is of importance for model-data fusion in carbon cycling studies and the accurate evaluation of ecosystem carbon budgeting. In this paper, a comprehensive analysis was conducted to investigate the influence of data processing procedures, focusing especially on the nocturnal data correction and three procedures in nonlinear regression method of gap filling [i.e., the selection of respiration model (REM), light-response model (LRM) and parameter optimization criteria (POC)], on the annual net ecosystem CO<sub>2</sub> exchange estimation at three forest ecosystems in China-FLUX with three yearly datasets for each site. The results showed that uncertainties caused from four methodological uncertainties were between 61 and 108 g C m<sup>-2</sup> year<sup>-1</sup>, with 61–93 g C m<sup>-2</sup> year<sup>-1</sup> (21–30%) in a temperate mixed forest, 80–107 g C m<sup>-2</sup> year<sup>-1</sup> (19–21%) in a subtropical evergreen coniferous plantation and 77–108 g C m<sup>-2</sup>

year<sup>-1</sup> (16–19%) in a subtropical evergreen broad-leaved forest. Factorial analysis indicated that the largest uncertainty was associated with the choice of POC in the regression method across all sites in all years, while the influences of the choice of models (i.e., REM and LRM) varied with climate conditions at the measurement station. Furthermore, the uncertainty caused by data processing procedures was of approximately the same magnitude as the interannual variability in the three sites. This result stressed the importance to understand the uncertainty caused by data processing to avoid the introduction of artificial between-year and between-site variability that hampers comparative analysis.

**Keywords** ChinaFLUX · Data processing · Eddy covariance · Net carbon exchange · Uncertainty

## Introduction

Eddy covariance (EC) observations of net ecosystem CO<sub>2</sub> exchange (NEE) have been analyzed to improve our knowledge of mechanisms and processes associated with the global carbon cycle (Hollinger et al. 1994; Baldocchi 2003, 2008). However, because of deficiencies in measurement and simulation technologies, more attention needs to be paid to the uncertainties inherent in these EC observations (Hollinger and Richardson 2005; Richardson et al. 2006; Lasslop et al. 2008; Wang et al. 2009). Increased knowledge of uncertainties in flux data will play a critical role in validating the use of various ecosystem models (e.g., Thornton et al. 2002; Churkina et al. 2003), synthesis research at multiple sites (e.g., Law et al. 2002; Churkina et al. 2005), and extrapolating flux data from the regional to the continental scale. However, the lack of knowledge about possible errors and uncertainties of EC

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observation is still one of the outstanding issues to be solved (Mauder et al. 2008).

There are different sources of uncertainties in the NEE flux observations. Hollinger and Richardson (2005) put forward a method for quantifying random errors in EC data by using the paired observations at two nearby towers or at equivalent environmental conditions in successive days. Subsequently, many studies on random measurement error have been carried out (Rannik et al. 2006; Richardson et al. 2006; He et al. 2010). In addition, as the EC data quality was usually influenced by instrumentation limits and the meteorological conditions, a series of post-field data processing and calculation, including footprint analyzing (Gockede et al. 2004, 2006), energy balance closure (Wilson et al. 2002; Foken 2008), data quality control (Foken and Wichura 1996) and gap filling (Falge et al. 2001; Ruppert et al. 2006), should be conducted before interpreting and analyzing the ecological meaning of EC observations. A set of data processing procedures and software have now been formed and are widely used for EC tower stations around the world (Reichstein et al. 2005; Papale et al. 2006; Mauder et al. 2008). However, at present, the method and parameter setting for each procedure are not identical. There is still a high heterogeneity in terms of quality and methods used in data processing across sites. It has been shown that even processing methods of internationally well-established experimental groups can result in significantly different values (Mauder et al. 2007). Therefore, in-depth knowledge of the impact of data processing procedures on NEE estimation is crucial if valid statistical comparisons are to be made across sites or across time. The influence of coordinate rotation, storage calculation, gap filling method selection on annual NEE estimation are now well known (Hollinger et al. 1994; Zhu et al. 2005; Papale et al. 2006; Moffat et al. 2007). However, the integral impact of critical data processing procedures, especially for the processing of nighttime data and the gap filling procedures, are still debatable and need further analysis.

Forest ecosystems play an important role in global carbon balance due to their large carbon storage and exchange (Valentini et al. 2000; Gower 2003). It is particularly important to derive accurate estimation of the carbon exchange of forested ecosystems. Our objective in the present paper was to use data from three forest sites within the ChinaFLUX network to conduct a comprehensive analysis of the uncertainty of annual NEE estimation associated with methodological uncertainties introduced by the data processing procedures. We focused on the influences of nocturnal data correction (NDC) and nonlinear regression method of gap filling. The uncertainty caused by NDC was evaluated by simulating the effect of friction velocity ( $u^*$ ) threshold selection on NEE determination with a bootstrapping approach. The impacts of gap filling strategies with nonlinear regression method were considered in three ways: (1) the selection of respiration model (REM); (2) the selection of light-response model (LRM); and (3) the selection of parameter optimization criteria (POC). By conducting this analysis, we could identify the relative influence of individual processing procedure and examine the interaction effect of different processing procedures on annual NEE estimation.

## Materials and methods

### Data and processing overview

In this study, we used observed half-hourly CO<sub>2</sub> flux and meteorological data collected from 2003 to 2005 at three ChinaFLUX forest sites: Changbaishan temperate broad-leaved Korean pine mixed forest (CBS), Qianyanzhou subtropical *Pinus* plantation (QYZ), and Dinghushan subtropical evergreen broad-leaved forest (DHS). The instruments for CO<sub>2</sub> flux and meteorological measurements at the three forest sites were described in Yu et al. (2006). The characteristics of the three sites are listed in Table 1. More detailed information at the three sites has been provided by

**Table 1** Site characteristics of the three forested CO<sub>2</sub> flux-tower stations in China

Site	CBS	QYZ	DHS
Location	42°24'N 128°06'E	26°44'N 115°03'E	23°10'N 112°34'E
Elevation (m)	738	100	300
Canopy height (m)	26	11	15
Mean temperature (°C)	3.6	17.9	20.9
Mean annual Precipitation (mm)	713	1,542	1,956
Dominant species	<i>Pinus koriaensis</i> <i>Tilia amurensis</i>	<i>Pinus massoniana</i> <i>Pinus elliottii</i> Engelm	<i>Schima superba</i> <i>Castanopsis chinensis</i>
Measurement height (m)	40	39	27

Guan et al. (2006), Wen et al. (2006), and Zhang et al. (2006a).

We used the ChinaFLUX flux data processing system (Li et al. 2008) to conduct quality control of the EC data. After a common quality checking process (triple coordinate rotation, WPL correction, de-spike, absolute value and storage change), fluxes with low  $u^*$  during nighttime were screened out (Reichstein et al. 2005). Data gaps were unavoidable in long-term and continuous measurements. Small gaps (<2 h) were linearly interpolated, while larger gaps were filled by the nonlinear regressions method as described in “Gap filling methods”.

Our goal in this study was to present a comprehensive analysis about the influence of NDC and nonlinear regression method of gap filling on the estimation of annual NEE. Therefore, we chose three possible  $u^*$  thresholds for each site in each year (5, 50 and 95% percentiles of  $u^*$  thresholds distribution obtained by a bootstrapping approach) to examine the effect of uncertainty in  $u^*$  threshold determination on annual NEE estimation. We applied two groups of simple but commonly used models for respiration and daytime NEE and assumed two error distributions of flux data that influence the implementation of model parameter optimization (Gaussian and double-exponential distribution) to illustrate the effect of gap filling procedures (i.e., non-linear regression method) on annual NEE estimation. In the following sections, we discuss the details of these cases and the analysis method.

#### Nocturnal data correction

Eddy flux measurements can underestimate the NEE during periods with low turbulence and thus limited air mixing. The friction velocity ( $u^*$ ) is currently used as a criterion to discriminate low and well mixed periods, and all data acquired during nighttime under low turbulent conditions were dismissed based on a  $u^*$  threshold criterion (Aubinet et al. 2000). In this study, we derived the  $u^*$  threshold for each site in each year by evaluating the relationship between temperature and  $\text{CO}_2$  flux as described in Reichstein et al. (2005) and Papale et al. (2006). Specifically, for the determination of  $u^*$  threshold, the dataset was split into six temperature classes of equal sample size and, for each temperature class, the set was then split into 20 equally sized  $u^*$  classes. When the nighttime flux reaches more than 99% of the average flux at the higher  $u^*$  classes, the threshold could be defined as the  $u^*$  class. The threshold was only accepted if, for the temperature class, temperature and  $u^*$  were not or only weakly correlated ( $|r| < 0.4$ ). The final threshold was defined as the median of the thresholds of the six temperature classes. This procedure was applied to the subsets of four 3-month periods to account for seasonal variation of vegetation

structure. For each period, the  $u^*$  threshold was reported, but the whole dataset was filtered according to the highest threshold found. In cases where no  $u^*$  threshold could be found, it was set to  $0.4 \text{ m s}^{-1}$ . A minimum threshold was set to  $0.1 \text{ m s}^{-1}$  for forest canopies in this study.

The procedure was repeated 1,000 times with a bootstrapping technique to assess the uncertainty of  $u^*$  threshold detection. In the bootstrapping procedure, a synthetic dataset was generated by randomly selecting  $n$  data points from the original dataset, which was itself of size  $n$ . In each bootstrapping step, the whole year was sampled on a half-hourly basis into a dataset with 17,520 or 17,568 data points, where each half-hour point could be drawn several times; some of the original data points would appear two or more times, and some of the original data points would not appear at all. The effect of missing data was also included since missing data are a sample with the same probability. Because resampling was done with replacements, each synthetic dataset would be different from the original dataset. The advantage of the bootstrapping was that parameters could be estimated without assumptions about the normal distribution and also using small sample sizes. The bootstrapping method can provide a non-parametric estimate of the  $u^*$  threshold uncertainty that otherwise is hard to obtain. Bootstrapping or similar sampling technique could provide an uncertainty estimate of the  $u^*$  threshold, which represented an important improvement over methods just providing a point estimate (Gu et al. 2005).

The 5 and 95% percentiles of the 1,000 bootstrapped threshold estimates were taken as confidence interval boundaries. And the 5, 50 and 95% percentiles were taken as the three supposed  $u^*$  thresholds to analyze the influence of the uncertainty in  $u^*$  threshold determination on annual NEE estimation.

#### Gap filling methods

In this study, the half-hourly  $\text{CO}_2$  flux data gaps were filled with the nonlinear regression method. So far, there are no standardized nonlinear regression methods across sites (Falge et al. 2001; Papale et al. 2006), and yet the choice of model, or how it is fitted, may have a significant effect on the fitted model parameters, and hence the model predictions. Therefore, in this study, two REM (considering the influence of temperature on respiration vs. considering the influence of temperature and soil moisture together), two LRM (i.e., the Michaelis–Menten model vs. its modification considering the effect of water condition), and two POC (i.e., minimizing the sum of squared deviations vs. minimizing the sum of absolute deviations) were used to examine the influence of gap filling strategies on NEE prediction.

## REM

During nighttime, there is no photosynthetic uptake and ecosystem respiration ( $R_e$ ) is the only source of NEE. Temperature and soil water availability are two important environmental variables regulating ecosystem respiration. Here, we used two simple but commonly used models to estimate the carbon exchange during nighttime with a yearly interval (Liu et al. 2009). The first model was Lloyd–Taylor (Eq. 1) which represented temperature effects on ecosystem respiration (Lloyd and Taylor 1994). The second one we used was a  $Q_{10}$  model described as a function of soil temperature and soil moisture (“ $Q_{10}$ – $S_w$ ”) (Eq. 2; Reichstein et al. 2002).

$$R_e = R_{e,ref} e^{E_0 \left( \frac{1}{T_{ref}-T_0} - \frac{1}{T_{soil}-T_0} \right)} \quad (1)$$

$$R_e = R_{e,ref} Q_{10}(S_w)^{\frac{(T_{soil}-T_{ref})}{10}} \quad Q_{10}(S_w) = a + bS_w \quad (2)$$

where  $R_e$  is the ecosystem respiration ( $\text{mg CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ ),  $R_{e,ref}$  is the ecosystem respiration ( $\text{mg CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ ) at the reference temperature ( $T_{ref}$ ), which is set to  $15^\circ\text{C}$  in this study, i.e.,  $288.15 \text{ K}$ ,  $E_0$  is the activation energy,  $T_0$  is the soil temperature when the ecosystem is equal to zero and is kept constant at  $-46.02^\circ\text{C}$  (i.e.,  $227.13 \text{ K}$ ) as in Lloyd and Taylor (1994),  $T_{soil}$  is soil temperature ( $^\circ\text{C}$ ),  $S_w$  is soil water content ( $\text{m}^3 \text{ m}^{-3}$ ) at  $5 \text{ cm}$  depth,  $a$  and  $b$  are fitted parameters. A positive value of  $b$  indicates that the temperature sensitivity of ecosystem respiration increases with increasing soil water content.

## LRM

For the daytime data, the response of NEE to photosynthetic photon flux densities (PPFD) was described as a rectangle hyperbola curve known as the Michaelis–Menten model (Eq. 3; Falge et al. 2001), with parameters fit at a 10-day time-step.

$$NEE = \frac{\alpha Q_{PPFD} P_{max}}{\alpha Q_{PPFD} + P_{max}} - R_e \quad (3)$$

where  $\alpha$  is the ecosystem photosynthetic photon yield ( $\text{mg CO}_2 \mu\text{mol photon}^{-1}$ ),  $Q_{PPFD}$  is the incident photosynthetic photon flux density ( $\mu\text{mol photon m}^{-2} \text{ s}^{-1}$ ),  $P_{max}$  is the maximum photosynthetic rate ( $\text{mg CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ ),  $R_e$  is the daytime ecosystem respiration ( $\text{mg CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ ).

The modification of the Michaelis–Menten model took into account the vapor pressure deficit (VPD) limitation of gross primary production (GPP) (“Michaelis–Menten–VPD”; Eq. 4). The parameter  $P_{max}$  in Eq. 3 was replaced with an exponentially decreasing function for  $P_{max}$  at high VPD (Lasslop et al. 2010):

$$P_{max} = \begin{cases} P_{max0} \exp(-k(\text{VPD} - \text{VPD}_0)), & \text{VPD} > \text{VPD}_0, \\ P_{max} = P_{max0}, & \text{VPD} < \text{VPD}_0. \end{cases} \quad (4)$$

The VPD in the atmosphere is used here.  $P_{max0}$  is the maximum photosynthetic rate that was not limited by VPD ( $\text{mg CO}_2 \text{ m}^{-2} \text{ s}^{-1}$ ),  $k$  is the response of the maximum carbon uptake to VPD, and  $\text{VPD}_0$  is set to  $10 \text{ hPa}$  when optimizing the model parameters.

## Parameter optimization criteria

Model parameter estimation can be described as varying the parameters until the best fit between model and data is found (Lasslop et al. 2008). The characteristic of the random flux error is the foundation of the implementing the model parameter optimization. Most models fitting to date had been based on the optimization criteria of ordinary least square method by minimizing the sum of squares, which can yield the maximum likelihood estimation when the random measurement error is normally distributed and homoscedastic (Richardson and Hollinger 2005). However, there is evidence that errors associated with eddy flux observation are better represented by a double-exponential distribution than a normal (Gaussian) distribution (Hollinger and Richardson 2005; Hagen et al. 2006; Richardson et al. 2006; Liu et al. 2009; He et al. 2010). In order to demonstrate the influence of the parameter optimization method on annual NEE, we performed an analysis with the two types of regression models of respiration and daytime NEE, considering in each case both an underlying Gaussian and an underlying double-exponential distribution.

We altered our assumption of how the error is distributed by specifying the form of the cost function ( $F_c$ ) that is minimized in the optimization routine. When assuming a Gaussian error distribution, we minimized the usual least squares error function (LS; Eq. 5). In the case of the double-exponential distribution assumption, we minimized the absolute deviations (AD; Eq. 6), based on the recommendation of Richardson and Hollinger (2005).

$$F_{C\_LS} = \sum_{i=1}^N \left( \frac{|y_i - y_{pred}|}{\sigma_i} \right)^2 \quad (5)$$

$$F_{C\_AD} = \sum_{i=1}^N \left( \frac{|y_i - y_{pred}|}{\sigma_i} \right) \quad (6)$$

where  $y_i$  is the measured data,  $y_{pred}$  is the model prediction,  $\sigma_i$  is the standard deviation of the random errors.

Given the fact that there are very few sites where two adjacent towers can simultaneously measure fluxes for the same ecosystem in ChinaFLUX, we used the daily-differencing approach as described by Hollinger and Richardson

(2005) and Richardson et al. (2006) to quantify the random flux errors. Specifically, a measurement pair ( $x_1$ ,  $x_2$ ) was considered valid only if both measurements were made under “equivalent” environmental conditions (i.e., PPFD within  $75 \mu\text{mol m}^{-2} \text{s}^{-1}$ , air temperature within  $3^\circ\text{C}$ , and wind speed within  $1 \text{ m s}^{-1}$ ) in the same successive 2 days. The daily-differenced paired fluxes  $((x_1 - x_2)/\sqrt{2})$  was used to express the inferred random flux error, and the error distribution and standard deviation ( $\sigma$ ) for each site in each year could be calculated. With the daily-differencing method, it was observed that random flux errors vary among sites. We found that the standard deviations of the random flux error exhibit distinct seasonal patterns in three forested sites. Meanwhile, the standard deviation for random flux errors in QYZ during the study period ( $\sigma = 0.203 \text{ mg CO}_2 \text{ m}^{-2} \text{s}^{-1}$ ) was larger than that in CBS ( $\sigma = 0.135 \text{ mg CO}_2 \text{ m}^{-2} \text{s}^{-1}$ ) and DHS ( $\sigma = 0.119 \text{ mg CO}_2 \text{ m}^{-2} \text{s}^{-1}$ ), which was of comparable magnitude to what has been estimated in AmeriFlux sites (Richardson et al. 2006).

### Uncertainty analysis

To quantify the uncertainty caused by four processing procedures considered in this study (i.e., NDC, REM, LRM and POC), the following steps were conducted:

In step 1, the yearly datasets were filtered with three  $u^*$  thresholds obtained in the section of NDC. There were three datasets corresponding three  $u^*$  thresholds for each site in each year. After that, eight combinations of gap filling procedures described in section of gap filling method (two LRM, two REM and two optimization methods) were used to fill the data gaps in each dataset, and 24 sets of complete time series of NEE were produced. Twenty-four annual NEE were estimated for each site in each year by summing the complete time series of NEE.

In step 2, the resulted 24 annual NEE obtained with different combinations of the correction and gap-filling methods were used as indicators of the methodological variability to analyze the effect of different processing method on the annual balance. In order to analyze the influence of single procedure on annual NEE, we split the 24 annual NEE into two or three groups according to the option of each procedure. There were 8 or 16 repetitions for each option of each procedure. Based on these repetitions, we considered the averaged value as the resulted annual NEE from the specified option of the procedure. We characterized the uncertainty of each procedures on annual NEE estimation by the maximum deviation of the mean annual NEE of groups for each single processing procedure to provide a clear quantitative information about the effect on the annual budget.

In step 3, analysis of variance was used to quantify the comprehensive influence of different procedures on the estimations of annual NEE. By this analysis, we could

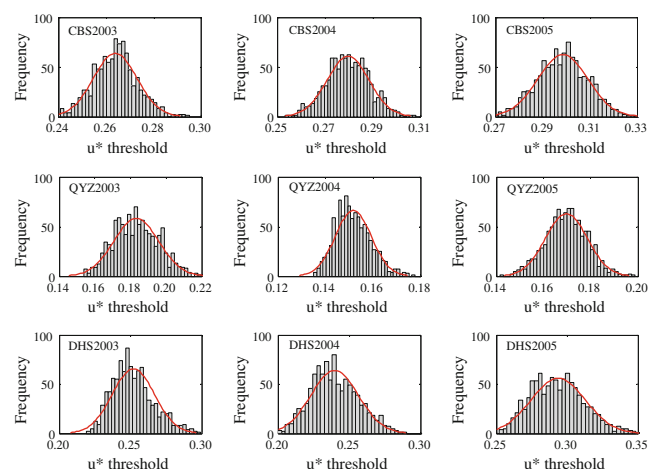
identify the relative influence of individual processing procedure and examine the interaction effect of different processing procedures on annual NEE estimation.

## Results and discussion

### Uncertainty of $u^*$ threshold values and its influence on NEE

By bootstrapping the annual datasets, we obtained the probability distribution and uncertainty of  $u^*$  thresholds (Fig. 1). For three yearly datasets for each site, the potential  $u^*$  threshold were generally normally distributed, and the 90% probability of the distribution could be considered as the confidence interval. Figure 2 demonstrates the estimated 90% confidence intervals for  $u^*$  threshold values at the three forest sites, which varied between 0.14 and  $0.33 \text{ m s}^{-1}$ . Note that the  $u^*$  thresholds were different across sites, with low values and uncertainty in QYZ and high values and uncertainty in DHS. This variability could be related to the characteristic of the site, such as canopy structure that affects the capacity of the eddies to penetrate in the forest, and topography that is one of the factors responsible for advection (Papale et al. 2006). Further analysis are needed to better understand the variability in the  $u^*$  threshold between sites.

The  $u^*$  correction had been applied to nighttime data in this study. However, there is still a debate on this, with part of the scientific community that applied the  $u^*$  correction to daytime and nighttime data (Papale et al. 2006). The amount of data removed by  $u^*$  correction varied across all sites and years as depicted in Table 2. The “missing” column indicated the percentage of missing NEE values with data not measured or deleted due to evident technical

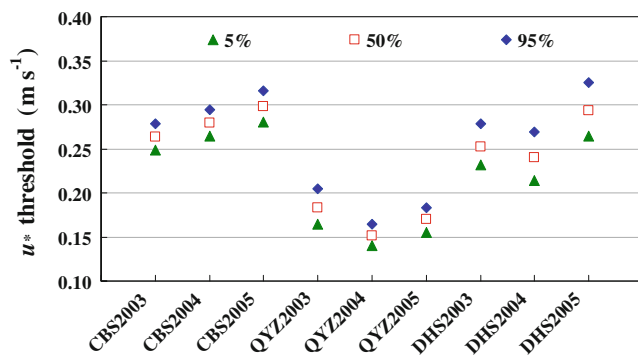


**Fig. 1** The distributions of the  $u^*$  threshold with bootstrapping approach for each site in each year



problems and spike detection. The three “ $u^*$ ” columns in Table 2 were the percentage of additional removal of data acquired under stable conditions according to the three thresholds used. A 10.9–22.0% of the annual data was excluded by the  $u^*$  correction, and the difference of the amount of data filtered by different  $u^*$  threshold was 1.2–2.6%.

As the  $u^*$  correction had been applied to only nighttime data, the absolute magnitude of the effect of  $u^*$  correction on annual NEE was equal to that on nighttime NEE. We found that the influence of NDC on the annual sum of NEE for all datasets analyzed here was  $14.8 \text{ g C m}^{-2} \text{ year}^{-1}$  on average, ranging from 5.8 to  $22.4 \text{ g C m}^{-2} \text{ year}^{-1}$  (Fig. 3), while the estimated value presented by Papale et al. (2006) was  $40 \text{ g C m}^{-2} \text{ year}^{-1}$ .



**Fig. 2** The 5, 50 and 95% percentiles of the  $u^*$  threshold distribution determined by the bootstrapping algorithm for the three yearly datasets at three sites

**Table 2** Percentage of net ecosystem  $\text{CO}_2$  exchange data that were missing and excluded by  $u^*$  correction for three forested sites from ChinaFLUX during 2003–2005

*Missing* percentage of data not measured or deleted due to evident technical problems and spike detection;  *$u^*$*  additional data removed due to low  $u^*$  conditions according with the three different  $u^*$  threshold during nighttime; *Total* the percentage of data removed summing missing data and  $u^*$  50%

The two numbers in italic are the percentages of nighttime and daytime, respectively, for each site in each year. All the percentages are relative to the year

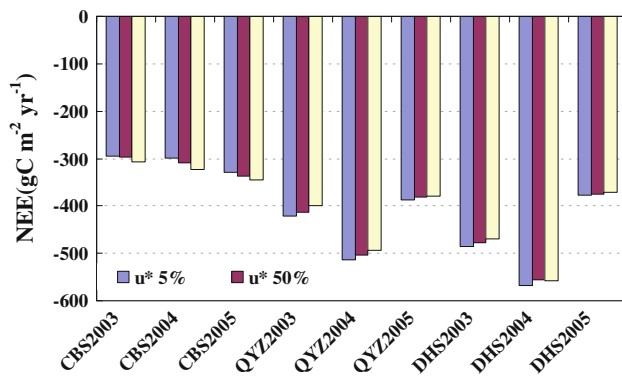
Site_year	Missing	<i><math>u^*</math> 5%</i>	<i><math>u^*</math> 50%</i>	<i><math>u^*</math> 95%</i>	Total
CBS2003	35.3	23.5	14.7	15.5	50.8
		<i>11.8</i>			<i>11.8</i>
CBS2004	43.4	26.2	12.6	13.3	56.7
		<i>17.2</i>			<i>17.2</i>
CBS2005	41.7	26.7	10.9	11.6	53.3
		<i>15.0</i>			<i>15.0</i>
QYZ2003	31.9	21.3	19.8	20.7	52.6
		<i>10.6</i>			<i>10.6</i>
QYZ2004	31.9	22.3	20.4	21.2	53.1
		<i>9.6</i>			<i>9.6</i>
QYZ2005	34.2	22.8	19.4	20.1	54.3
		<i>11.4</i>			<i>11.4</i>
DHS2003	44.6	25.8	14.0	14.9	59.5
		<i>18.8</i>			<i>18.8</i>
DHS2004	54.5	30.4	11.3	12.2	66.7
		<i>24.1</i>			<i>24.1</i>
DHS2005	37.8	23.1	12.4	13.7	51.5
		<i>14.7</i>			<i>14.7</i>

The difference could be related to the range of the 5 and 95% percentiles, while the  $u^*$  threshold at three forested sites in this study was  $0.14\text{--}0.33 \text{ m s}^{-1}$ , smaller than those reported in eight sites in Europe ( $0.1\text{--}0.7 \text{ m s}^{-1}$ ). It could also be seen in Fig. 3 that the annual NEE estimation decreased with increasing  $u^*$  threshold as expected at QYZ and DHS. It could be explained by the fact that the observed carbon fluxes increased under high turbulence conditions, which implied that the magnitude of the valid nighttime fluxes increased with the  $u^*$  threshold, i.e. high annual respiration and low NEE. In contrast to the decreasing trend with increasing  $u^*$  threshold in QYZ and DHS, the relationship between the  $u^*$  threshold and annual NEE showed an increasing tendency in CBS. The increasing tendency in CBS may related to that reported in Zhang et al. (2005), in which the result showed that nighttime NEE decreases, even negative, with increasing wind speed when  $u^* > 0.25$  in CBS. When we used these data excluding the higher  $u^*$  threshold to fill the ecosystem respiration, a lower annual respiration and a higher NEE is produced.

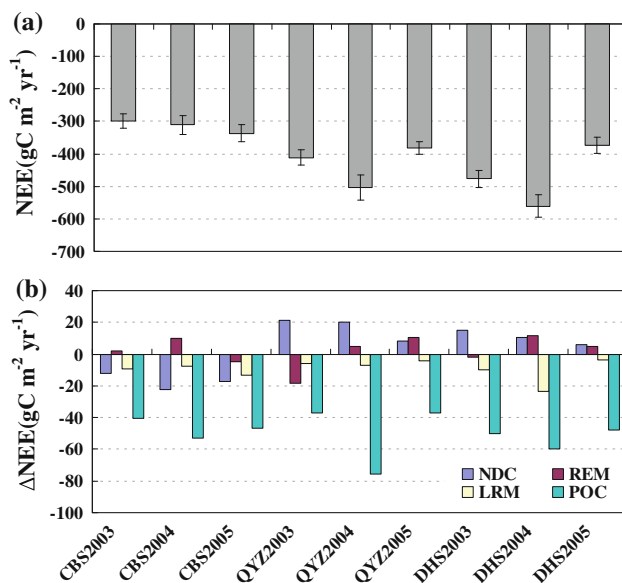
#### Impacts of the gap-filling procedures

##### *Influence of REM*

The uncertainty caused by REM on annual NEE varied across sites, ranging from  $1.8 \text{ g C m}^{-2} \text{ year}^{-1}$  at DHS and  $18.3 \text{ g C m}^{-2} \text{ year}^{-1}$  at QYZ (Fig. 4). This uncertainty was significantly correlated with the environment conditions of the tower station. For example, the highest



**Fig. 3** Effect of nocturnal data correction on annual net ecosystem  $\text{CO}_2$  exchange (NEE). The annual NEE for each  $u^*$  threshold was averaged from the corresponding eight annual NEE estimations with two REM, two LRM and two parameter optimization criteria ( $2 \times 2 \times 2$ ) for each site in each year



**Fig. 4** Effects of four factors on the estimation of annual net ecosystem  $\text{CO}_2$  exchange (NEE). **a** Total estimation and bias of annual NEE, **b** Bias introduced by different processing procedures on annual NEE. *NDC* the influence of the determination of  $u^*$  threshold for nocturnal data correction (the results from 95%  $u^*$  threshold minus that from 5%  $u^*$  threshold), *REM* the influence of respiration model (the results from  $Q_{10}-S_w$  minus that from Lloyd–Taylor model), *LRM* the influence of light-response model selection (the results from the Michaelis–Menten–VPD model minus that from the Michaelis–Menten model), *POC* the influence of parameter optimization criteria (the results from absolute deviation criteria minus that from ordinary least squares criteria)

uncertainty of REM occurred in QYZ during 2003, largely due to a severe drought occurred during the summer of 2003 (Liu et al. 2005). The effect of the drought stress on CBS and DHS was not as apparent as that on QYZ due to the abundant rainfall and mild temperature (Zhang et al. 2006b).

Furthermore, when the soil water availability effect was not included in the respiration modeling, the resultant annual NEE magnitude was smaller than that obtained from the model considering water effect except for CBS in 2005, QYZ in 2003 and DHS in 2003, where the changes were in the opposite direction (Fig. 4). This could be related to the drought stress in the first half year of 2005 in CBS, the summer of 2003 in QYZ and the year-end of 2003 in DHS. The performance of the two REM varied from site to site. Regardless of the optimization criterion used, the performance of REM was equivalent among different sites (see Table 3, exemplary for the CBS site in 2003), while for QYZ with perennial summer drought, especially an abnormal drought in 2003, the fit was significantly increased by considering the effect of water availability on ecosystem respiration.

#### Influence of LRM

By grouping the 24 results of annual NEE datasets according to the LRM into two class, we could calculate the uncertainty of annual NEE that caused by LRM selection as the difference of the averaged value of each class. The result showed that, for the three yearly datasets of the three sites used in this study, the uncertainty caused by LRM on annual NEE estimation was  $3.5\text{--}23.6 \text{ g C m}^{-2} \text{ year}^{-1}$ , with  $7.8\text{--}13.2 \text{ g C m}^{-2} \text{ year}^{-1}$  in CBS,  $4.4\text{--}7.3 \text{ g C m}^{-2} \text{ year}^{-1}$  in QYZ and  $3.5\text{--}23.6 \text{ g C m}^{-2} \text{ year}^{-1}$  in DHS (Fig. 4).

It was possible to see that when the VPD effect was not included in a light-response curve (i.e., Michaelis–Menten), the resultant annual NEE magnitude were smaller than that from the model considering VPD effect (i.e., Michaelis–Menten–VPD). The decrease of NEE magnitude could be caused by a limitation of GPP due to stomatal closure at high VPDs (Lasslop et al. 2010). Meanwhile, regardless of the optimization criterion used, the modified Michaelis–Menten model considering VPD performed better than the original Michaelis–Menten model (see Table 4, exemplary for the QYZ site in 2003, day of year: 181–190), with higher value of  $R^2$  and root mean squared error (RMSE) when including VPD in the model. It implied that including a VPD limitation of daytime carbon exchange in the model improved the ability of the model to reproduce the carbon exchange condition. The results also showed that the Michaelis–Menten model during gap filling might underestimate the annual NEE magnitude, and the model including VPD could eliminate the clear systematic bias.

As the effect of model selection for gap filling on annual NEE estimation could be considered as the different simulations of the missing data, it was possible to expect that the uncertainty due to light response selection increased with the increasing of the percentage of missing

**Table 3** Estimates of the parameters of respiration for CBS in 2003, described by the Lloyd–Taylor and  $Q_{10}$ – $S_w$  model with different parameter optimization criteria with observations filtered by 50%  $u^*$  threshold

	$R_{e,ref}$ (mg CO <sub>2</sub> m <sup>-2</sup> s <sup>-1</sup> )	$E_0$ (K) or $a$	$b$	$R^2$	RMSE (mg CO <sub>2</sub> m <sup>-2</sup> s <sup>-1</sup> )	MAE (mg CO <sub>2</sub> m <sup>-2</sup> s <sup>-1</sup> )
Lloyd–Taylor						
Least square criteria	0.2772	389.93		0.58	0.0942	0.0581
Absolute deviation criteria	0.2572	439.23		0.58	0.0953	0.0563
$Q_{10}$ – $S_w$						
Least square criteria	0.2689	3.89	–2.2661	0.58	0.0951	0.0589
Absolute deviation criteria	0.2508	4.65	–6.5832	0.57	0.0968	0.0559

RMSE root mean squared error, MAE mean absolute error

**Table 4** Estimates of the parameters of the carbon exchange during daytime for QYZ, 2003, day of year: 181–190, described by the Michaelis–Menten and Michaelis–Menten–VPD models with different parameter optimization criteria

	$\alpha$ (mg CO <sub>2</sub> μmol photon <sup>-1</sup> )	$P_{max}$ or $P_{max0}$ (mg CO <sub>2</sub> m <sup>-2</sup> s <sup>-1</sup> )	$k$	$R_e$ (mg CO <sub>2</sub> m <sup>-2</sup> s <sup>-1</sup> )	$R^2$	RMSE (mg CO <sub>2</sub> m <sup>-2</sup> s <sup>-1</sup> )	MAE (mg CO <sub>2</sub> m <sup>-2</sup> s <sup>-1</sup> )
Michaelis–Menten							
Least square criteria	0.0019	1.0568		0.2642	0.83	0.1051	0.0805
Absolute deviation criteria	0.0016	1.0225		0.2232	0.83	0.1060	0.0799
Michaelis–Menten–VPD							
Least square criteria	0.0014	1.8078	0.0276	0.2364	0.85	0.0987	0.0737
Absolute deviation criteria	0.0015	1.5849	0.0013	0.2240	0.86	0.0990	0.0722

VPD vapor pressure deficit, RMSE root mean squared error, MAE mean absolute error

daytime data. For example, for DHS in 2004, the relative higher effect might be associated with the higher percentage of missing daytime NEE data, which was 24.1% compared with 9.6–18.8% in other sites and years (see Table 2).

#### Influence of parameter optimization criteria

The use of absolute deviation in the cost function was suggested previously by Richardson et al. (2006). Here, we used both least squares and absolute deviations to illustrate the effects of parameter estimation and model prediction. For our studied sites in different years, the choice of the optimization criterion (LS vs. AD) not only influenced the fitted model parameters but also the resultant model predictions (Tables 3 and 4). We compared model fit and model predictions using the two pairs of respiration and LRM. The results showed that the uncertainty caused by POC on annual nighttime NEE estimation (40.8–74.0 g C m<sup>-2</sup> year<sup>-1</sup>) was higher than that on daytime annual NEE estimation

(0.9–13.5 g C m<sup>-2</sup> year<sup>-1</sup>). Meanwhile, the modeled annual sum of NEE was always higher (37–76 g C m<sup>-2</sup> year<sup>-1</sup>) with the least squares criterion compared with the absolute deviation (Fig. 4), mainly resulting from the bias in the ecosystem respiration (90–168 g C m<sup>-2</sup> year<sup>-1</sup>). This could be related to the missing data percentage during nighttime and daytime. Up to 70% of nighttime data was missing after  $u^*$  correction, while the missing percentage for daytime data was usually below 40% (see Table 2).

The RMSE of AD increased compared to that of LS, while the mean absolute error (MAE) decreased, which was related to the optimization criterion (Tables 3 and 4). Furthermore, even with the similar model performance ( $R^2$ , RMSE and MAE), the two optimal criteria lead to different parameter sets, which then led to different model prediction. For example, for the Lloyd–Taylor model in CBS2003 (Table 3), the optimal LS parameters were  $R_{e,ref} = 0.2772$  mg CO<sub>2</sub> m<sup>-2</sup> s<sup>-1</sup>,  $E_0 = 389.93$  K. In contrast, the absolute deviation of model parameters had lower values of  $R_{e,ref}$  (0.2572 mg CO<sub>2</sub> m<sup>-2</sup> s<sup>-1</sup>) and

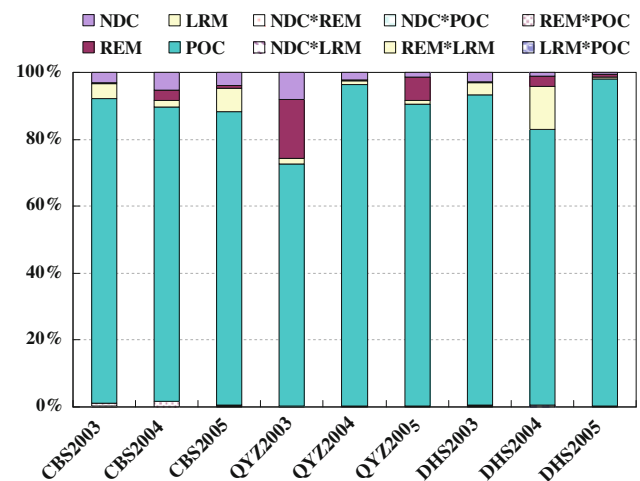


higher values of  $E_0$  (439.23 K). Note that, by now, there was not a uniquely defined, unambiguously optimal parameter set. In fact, what is meant by “optimal” in this context was somewhat subjective (e.g., Gupta et al. 1999; Richardson et al. 2010). The equifinality of the parameter optimization may be an important aspect in considering the difference in model prediction.

#### Comprehensive analysis of the data processing procedures

The annual NEE obtained with the different combinations of the four procedures (i.e., NDC, REM, LRM and POC) was used as indicators of the methodological variability to analyze the effect of the different procedures on the annual balance as illustrated in Fig. 4. In the lower panel, the ranges of annual NEE due to each single method were shown, while the upper panel plotted the mean annual NEE with an error bar indicating minimum and maximum values obtained for each site in each year. Looking at the annual NEE, it is possible to see that the uncertainties caused from four methodological uncertainties were between 61 and 108 g C m<sup>-2</sup> year<sup>-1</sup> and the relative uncertainty in general between 16 and 25%, except for CBS in 2004 where it was about 30%. The uncertainty caused by data processing procedures was of approximately the same magnitude of the interannual variability in the three sites. This result stressed the importance to understand the uncertainty caused by data processing to avoid the introduction of artificial between-year and between-site variability that hampers comparative analysis. Moreover, the POC in nonlinear regression method had the strongest impact on the NEE estimation, with an effect on the annual NEE of average 49.7 g C m<sup>-2</sup> year<sup>-1</sup>. QYZ in 2004 and DHS in 2004 were the sites with the highest parameter optimization effect on the annual NEE (QYZ 2004, 75.6 g C m<sup>-2</sup> year<sup>-1</sup>; DHS 2004, 59.9 g C m<sup>-2</sup> year<sup>-1</sup>), while for other sites like QYZ 2003 it was small.

To understand the relative role of different processing procedures in the total uncertainty, an analysis of variance was performed using the 24 annual NEE resulting for each site in each year (Fig. 5). The main source of uncertainty was confirmed to be POC for all sites in all years, the average effect of POC on annual NEE was 88.7%, range from 72.3% in QYZ2003 and 97.8% in DHS2005, while the effect of NDC, REM and LRM were 3.2, 3.7 and 3.9%, respectively. It was possible to see that the influence of NDC was relative stable among different sites in different year, which could be related to the small variability of the data percentage that was filtered with three  $u^*$  thresholds, while the variability of selection of REM and LRM were greater. This result indicated that the influence of optimization method and  $u^*$  filtering on annual NEE were somewhat intrinsic, and the influence of REM and LRM varied



**Fig. 5** Results of the analysis of variance test on the three yearly datasets of three forest sites. *NDC* determination of  $u^*$  threshold for nocturnal data correction, *REM* the selection of respiration model, *LRM* the selection of light-response model, *POC* the selection of parameter optimization criteria. Asterisks indicate comprehensive effects of two factors. Y-axis illustrates the relative role of different processing procedures in the total uncertainty

with the specific climate conditions of the site. Another important aspect was that the interaction effects between any two processing methods were very low, so that the four procedures seem to be independent from each other.

#### Conclusions

In this paper, we investigated the effects of data processing procedures, focusing especially on the NDC and three procedures in the nonlinear regression method of gap filling (i.e., the selection of REM, LRM and POC), on the annual NEE estimation at three forest ecosystems in ChinaFLUX with three yearly datasets for each site. The uncertainties caused by four processing procedures were between 61 and 108 g C m<sup>-2</sup> year<sup>-1</sup> with relative uncertainty in general between 16 and 25%. The main source of uncertainty was the determination of POC, accounting for an average effect of 88.7% on annual NEE. The influence of NDC was relative stable among all sites in all years, while the variability of selection of REM and LRM were greater according to the data missing percentage and climate condition. Moreover, we could conclude that the influence of NDC and POC on annual NEE were stable and intrinsic, while the influences of respiration and LRM varied with the specific conditions of the tower site. The results stressed the importance of making full knowledge of the specific conditions of the EC tower site and choosing the suitable procedures during EC data processing to avoid the introduction of artificial between-year and between-site variability that hampers comparative analysis.

The integral uncertainties during post-field data processing should be considered in any statistical analysis, process model evaluation, and model data fusion based on EC observation. Future work is needed to combine the potential uncertainty sources under a common framework, so that the total uncertainty of flux observation and estimation might be more accurately specified.

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