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## RESEARCH ARTICLE

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### Key Points:

- A mixed forest was observed as a larger CO<sub>2</sub> sink/source than a rice paddy due to a longer growing period and stronger ecosystem respiration
- The biogenic sink offsets about 70% of anthropogenic contribution to column-averaged CO<sub>2</sub> concentrations over Northeast China
- Uncertainty of simulated CO<sub>2</sub> fluxes with the WRF-VPRM largely depends on VPRM parameters, in particular maximum light use efficiency

### Supporting Information:

- Supporting Information S1

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## Terrestrial CO<sub>2</sub> Fluxes, Concentrations, Sources and Budget in Northeast China: Observational and Modeling Studies

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**Abstract** CO<sub>2</sub> fluxes and concentrations are not well understood in Northeast China, where dominant land surface types are mixed forest and cropland. Here, we analyzed the CO<sub>2</sub> fluxes and concentrations using observations and the Weather Research and Forecasting model coupled with the Vegetation Photosynthesis and Respiration Model (WRF-VPRM). We also used WRF-VPRM outputs to examine CO<sub>2</sub> transport/dispersion and budgets. Finally, we investigated the uncertainties of simulating CO<sub>2</sub> fluxes related to four VPRM parameters (including maximum light use efficiency, photosynthetically active radiation half-saturation value, and two respiration parameters) using off-line ensemble simulations. The results indicated that mixed forests acted as a larger CO<sub>2</sub> source and sink than rice paddies in 2016 due to a longer growth period and stronger ecosystem respiration, although measured minimum daily mean net ecosystem exchange (NEE) was smaller at rice paddy ( $-10 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) than at mixed forest ( $-6.5 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) during the growing season (May–September). The monthly fluctuation of column-averaged CO<sub>2</sub> concentrations (XCO<sub>2</sub>) exceeded 10 ppm in Northeast China during 2016. The large summertime biogenic sinks offset about 70% of anthropogenic contribution of XCO<sub>2</sub> in this region. WRF-VPRM modeling successfully captured seasonal and episodic variations of NEE and CO<sub>2</sub> concentrations; however, NEE in mixed forest was overestimated during daytime, mainly due to the uncertainties of VPRM parameters, especially maximum light use efficiency. These findings suggest that the WRF-VPRM modeling framework will provide greater understanding of the natural and anthropogenic contributions to the carbon cycle in China, especially after calibration of parameters that control biogenic fluxes.

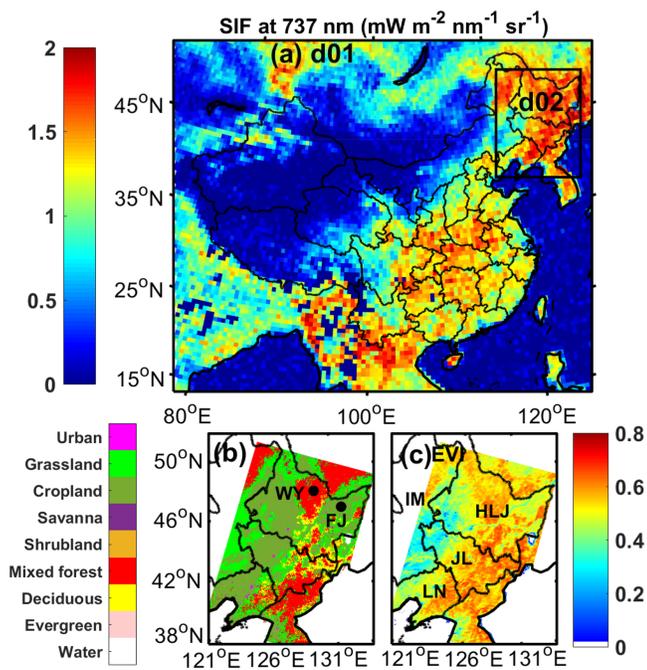
### 1. Introduction

Carbon dioxide (CO<sub>2</sub>), as one of the major greenhouse gases in the atmosphere, has been considered as a key driver for climate variability and change (Forster et al., 2007; Gregory et al., 2020; Szulejko et al., 2017). Increasing atmospheric CO<sub>2</sub> can produce warmer temperatures in the troposphere and cooler temperatures in the stratosphere, intensify the residual circulation from the equator to the pole, and even modify the chemistry of the future atmosphere (Rind et al., 1990; Seo et al., 2017; Singh et al., 2017). Globally averaged concentrations of atmospheric CO<sub>2</sub> have increased from 280 ppm since the Industrial Revolution (Bauska et al., 2015; Etheridge et al., 1996) to 403.3 ppm in 2016 (WMO, 2017). The growth rate of atmospheric CO<sub>2</sub> concentrations, which represents the additional burden of CO<sub>2</sub> for a given year integrated over all sources and sinks, remained about 2 ppm/year after 2010 (Keenan et al., 2016) but has been as large as 2.96 ppm/year in 2015 due to the tropical outgassing arising from the El Niño (Yue et al., 2017). On the global scale, the ocean and the terrestrial biosphere remove approximately 45% of the CO<sub>2</sub> emitted by human activities each year (Le Quéré et al., 2015), though the interannual variability in the global sink is large. Regional CO<sub>2</sub> sources/sinks have even larger uncertainties. The complex processes and interactions controlling CO<sub>2</sub> uptake/emission by land ecosystems are still not completely understood (Ciais et al., 2019; Reuter et al., 2017; Schimel et al., 2015).

Quantifying the CO<sub>2</sub> uptake by terrestrial ecosystems is significant for understanding the carbon cycle and budget and the real impact of anthropogenic emissions on the growth rate of atmospheric CO<sub>2</sub> concentrations (Dayalu et al., 2018). Various “top-down” and “bottom-up” approaches have been proposed to quantify terrestrial CO<sub>2</sub> fluxes on regional and global scales (Baldocchi et al., 1996; Basu et al., 2018; Knorr, 2000; Piao et al., 2013; Reuter et al., 2017). Atmospheric inversion is a commonly used method that applies an atmospheric transport model to infer the CO<sub>2</sub> fluxes between the land surface and the atmosphere based on in situ-observed and/or satellite-retrieved CO<sub>2</sub> spatiotemporal gradients (e.g., Crowell et al., 2018; Peylin et al., 2013). The inversion method relies on the accuracy of (1) the assumed prior flux field and its error structure, (2) the atmospheric transport modeling, (3) the observational data set assimilated, and (4) the assimilation technique (e.g., Engelen et al., 2004; Ciais et al., 2010). Therefore, there remain large differences among atmospheric-inversion estimates of terrestrial CO<sub>2</sub> fluxes (Basu et al., 2018; Crowell et al., 2019; Peylin et al., 2013; Zhang et al., 2014). Bottom-up methods simulate terrestrial ecosystem CO<sub>2</sub> fluxes using a process- or data-based biosphere model by considering the biochemical mechanisms and physical processes. For example, Tian et al. (2011) used a process-based ecosystem model driven by multiple and complex environmental factors to simulate the net ecosystem exchange (NEE) of CO<sub>2</sub> in China during 1961–2005. However, the environmental process parameters in process-based models are difficult to quantify on different scales (Shi et al., 2018; Zhu et al., 2005), as they are typically validated only at sparse sites over limited ecosystem types. Alternatively, satellite remote sensing presents an opportunity to provide data with global spatial coverage and so evaluates models in a greater variety of conditions. Remote-sensing data-driven models, especially the light use efficiency (LUE) models, have been developed and widely used to simulate the gross ecosystem exchange (GEE) and NEE from ecosystem to regional to global scales. The commonly used LUE models include the Carnegie-Ames-Stanford Approach (Field et al., 1995), Carbon Fix (Veroustraete et al., 2002), Carbon Flux (Turner et al., 2006), the Eddy-Covariance (EC)-LUE model (Yuan et al., 2007), the Vegetation Photosynthesis Model (Xiao et al., 2004), and the Vegetation Photosynthesis and Respiration Model (VPRM) (Mahadevan et al., 2008). GEE and NEE estimated using LUE models still have large uncertainties and discrepancies, mainly due to model structure differences (Yuan et al., 2014) and model parameter choices (Hilton et al., 2013). In general, top-down and bottom-up estimates differ widely across all spatiotemporal scales.

In order to reconcile estimates of NEE using top-down and bottom-up methods, researchers have been incorporating the in situ and satellite observations into modeling studies. The high-temporal-resolution EC measurements of CO<sub>2</sub> fluxes and concentrations over diverse biomes crossing wide latitudes have been widely applied to optimize model parameters and validate modeling results (Dayalu et al., 2018; Hilton et al., 2013; Jamroensan, 2013; Mahadevan et al., 2008; Yuan et al., 2014). In addition, column-averaged CO<sub>2</sub> concentrations (XCO<sub>2</sub>) retrieved from satellites are effective to constrain CO<sub>2</sub> fluxes and can be used to evaluate simulation results on wide spatial scales, especially in the regions with limited in situ measurements (Basu et al., 2013; Crowell et al., 2019; Hu et al., 2019b; Rayner et al., 2014; Rayner & O'Brien, 2001).

CO<sub>2</sub> flux distribution and variation are heavily influenced by meteorological conditions. Previous studies reported that the cyclones (Hurwitz et al., 2004; Zhou et al., 2017), cold fronts (Hu et al., 2019a), and sea-land (Ahmadov et al., 2007) and lake-land breezes (Diao et al., 2015) resulted in large fluctuations in atmospheric CO<sub>2</sub> fluxes and concentrations and played a major role in regional and global CO<sub>2</sub> transport and budget (Chan et al., 2004; Parazoo et al., 2011). Therefore, it is critical to develop a weather-biosphere fully coupled model to investigate the mutual impacts of different CO<sub>2</sub> sources and meteorological conditions on the spatiotemporal variation of atmospheric CO<sub>2</sub> concentrations. Ahmadov et al. (2007) coupled the VPRM into the Weather Research and Forecasting (WRF) model to simulate terrestrial CO<sub>2</sub> fluxes and their subsequent atmospheric transport in France. The subsequent study indicated that the WRF-VPRM was able to capture the atmospheric CO<sub>2</sub> temporal and spatial distributions and performed better than other global models in simulating diurnal variability of atmospheric CO<sub>2</sub> concentration field (Ahmadov et al., 2009). In the past decade, the application and evaluation of WRF-VPRM mainly focused on North America (Feng et al., 2016; Hu et al., 2019b; Park et al., 2018; Ye et al., 2017) and Europe (Pillai et al., 2011). The model performances remain unknown in Asia including China due to the lack of observations, as well as model uncertainties due to uncertainties of VPRM parameters in the region (Dayalu et al., 2018; Hilton et al., 2013; Liu et al., 2015; Zhang et al., 2017a). Diao et al. (2015) used WRF-VPRM to



**Figure 1.** (a) Domain configuration for the WRF-VPRM simulation with the first domain (d01) covering China and the second domain (d02) focusing on Northeast China including four provinces, that is, Heilongjiang (HLJ), Jilin (JL), Liaoning (LN), and the eastern part of Inner Mongolia (IM) Autonomous Region. The background shading shows the spatial distributions of  $0.5^\circ \times 0.5^\circ$  summertime (June, July, and August) Sun-induced Fluorescence (SIF) from the Global Ozone Monitoring Experiment-2 (GOME-2) in 2016, (b) dominant vegetation types, and (c) summertime enhanced index vegetation (EVI) in d02 derived from the Moderate Resolution Imaging Spectroradiometer (MODIS) satellite. Black dots represent locations of the rice paddy site in Fujin (FJ) and the mixed forest site in Wuying (WY).

investigate the spatiotemporal characteristics of NEE and surface  $\text{CO}_2$  concentrations over the Yangtze River Delta region in China for 5 days, from 28 July to 2 August 2010. Ye et al. (2017) assessed the biotic contribution to the  $\text{XCO}_2$  enhancements during two short episodes (12–15 January and 1–4 August 2015) over the Pearl River Delta metropolitan region in China using the WRF-VPRM. However, these short-term (a few days) simulations could not reveal long-term variations of  $\text{CO}_2$  fluxes/concentrations. Recently, Dayalu et al. (2018) simulated the NEE over different ecosystems in northern China during the growing seasons (May through September) in 2015–2017 based on the VPRM after optimizing four model parameters using EC measurements and then scaled up regionally using the WRF model in an off-line mode to assess the biotic contributions of atmospheric  $\text{CO}_2$  concentrations in this region. Nevertheless, the off-line simulation cannot capture the real-time feedback between synoptic weather and land-surface dynamics and leads to large uncertainties in the simulated  $\text{CO}_2$  fluxes/concentrations (Hu, 2008). Liu et al. (2018) reported that surface  $\text{CO}_2$  concentrations simulated with the WRF-VPRM exhibited a similar trend with those observed at the Shangdianzi station in Beijing from February to May in 2015. In sum, long-term simulations and observations of  $\text{CO}_2$  fluxes/concentrations required to investigate and quantify  $\text{CO}_2$  sources/sinks and budget in China are currently rarely reported (He et al., 2019; Thompson et al., 2016; Zhang et al., 2014).

Northeast China (latitudes ranging from  $40^\circ$ – $55^\circ\text{N}$ ), consisting of provinces of Heilongjiang, Jilin, and Liaoning, as well as the eastern Inner Mongolia Autonomous Region, has two dominant terrestrial ecosystems, cropland and mixed forest (Figure 1b). This region has strong terrestrial  $\text{CO}_2$  fluxes in China as indicated by the high Sun-induced Fluorescence (SIF) in summer (June, July, and August) from the Global Ozone Monitoring Experiment-2 (GOME-2) (Fig. 1a). SIF is a direct indicator of photosynthetic activity (Krause & Weis, 1991) and on ecosystem scales has been shown to be proportional to GEE (Sun

et al., 2018). Researchers have investigated the seasonal and diurnal variations of  $\text{CO}_2$  fluxes using EC measurements over different ecosystems in Northeast China, including rice paddy fields (Jia et al., 2017; Li et al., 2018; Liang et al., 2007), forest regions (Guan et al., 2006; Wang et al., 2008) as well as some less-dominant ecosystems like reed wetlands (Li et al., 2016; Zhou et al., 2009), and freshwater marshes (Yang et al., 2013; Zhang et al., 2005). The EC-measured  $\text{CO}_2$  fluxes over rice paddies and mixed forests show a distinct seasonal variation, with the largest  $\text{CO}_2$  drawdown (approximately dozens of  $\mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) occurring in summer due to strong ecosystem photosynthesis while remaining near zero in winter (Guan et al., 2006; Li et al., 2016; Song et al., 2006). Influenced by the seasonal variation of  $\text{CO}_2$  fluxes, the satellite-retrieved  $\text{XCO}_2$  exhibited higher values in spring and lower values in summer. Due to prominent terrestrial  $\text{CO}_2$  fluxes, the  $\text{XCO}_2$  in Northeast China exhibited a larger seasonal variation than in other regions in China (Xu et al., 2017; Yang et al., 2016). In addition,  $\text{CO}_2$  fluxes exhibited an obvious diurnal variation during the growing season, reaching a maximum sink in the middle of the daytime with a small efflux at night. Previous studies on  $\text{CO}_2$  fluxes mostly focused on a specific vegetation type but rarely compared among various dominant ecosystems and rarely examined their overall contribution to total  $\text{CO}_2$  budget in Northeast China.

Although researchers have been aware of the potential large impact of terrestrial  $\text{CO}_2$  fluxes on atmospheric  $\text{CO}_2$  in Northeast China, the detailed spatiotemporal characteristics of  $\text{CO}_2$  sources/sinks and budget are still not well understood in this region. Piao et al. (2009) reported that Northeast China was a net source of  $\text{CO}_2$  to the atmosphere owing to overharvesting and degradation of forest during 1980s and 1990s. However, Jiang et al. (2016) indicated that the  $\text{CO}_2$  uptake by land ecosystems has been increasing after the 1990s in China



Figure 2. Panoramic views of (a) the rice paddy site in Fujin and (b) mixed forest site in Wuying.

because warmer climate and higher levels of atmospheric CO<sub>2</sub> contributed to the increase of productivity in terrestrial ecosystems (Wu et al., 2014). Such a trend has also been reported in the Northern Hemisphere (Ciais et al., 2019) and northern Asia (Peylin et al., 2013). Diao et al. (2006) used an inverse Lagrangian dispersion assimilation technique to constrain the CO<sub>2</sub> source/sink by assimilating data from the Changbai Mountain forest station in Northeast China. However, they only studied one station rather than the whole area of Northeast China.

In this study, we utilize EC measurements, Orbiting Carbon Observatory-2 (OCO-2) satellite data set, and the online WRF-VPRM model to investigate the CO<sub>2</sub> fluxes, concentrations, sources/sinks, and atmospheric CO<sub>2</sub> budget, as well as the impacts of meteorological conditions on CO<sub>2</sub> variations. We also discuss the uncertainties of NEE simulations in relation to the choices of parameters in off-line VPRM simulations.

The rest of this paper is organized as follows. Section 2 introduces observational data and processing procedures and describes the WRF-VPRM model and simulation setup. Section 3 analyzes the seasonal and episodic variations of surface CO<sub>2</sub> fluxes and concentrations in major ecosystems (cropland and mixed forest) in Northeast China and then quantifies biogenic and anthropogenic contributions to XCO<sub>2</sub>. We also analyze the diurnal variations of surface CO<sub>2</sub> fluxes and concentrations and model

uncertainties of CO<sub>2</sub> fluxes associated with VPRM parameters. Conclusions are summarized in section 4.

## 2. Methods

### 2.1. Field Measurements

#### 2.1.1. Site Description

Cropland and mixed forest are major terrestrial ecosystems in Northeast China (Figure 1b). The cropland area in Northeast China was about 215,000 km<sup>2</sup>, accounting for 13.3% of the total cropland area in China (Xie et al., 2019). These croplands mostly distributed in plain regions, including the Sanjiang Plain, the Songnen Plain, and the Liaohe Plain. Rice is a major crop in this region, and rice paddy area has been increasing persistently since the 1980s, especially in the Sanjiang Plain (Wu et al., 2014). Forests, particularly mixed forests, cover about 394,500 km<sup>2</sup> area in Northeast China. The forest coverage rate in this region (40%) was more than twice that in China as a whole (16.5%) (Huang, 2019). Mixed forests in Northeast China are mostly located in mountain areas, including the Changbai Mountains, the Da Hinggan Mountains, and the Xiao Hinggan Mountains.

To investigate the CO<sub>2</sub> surface flux and concentration characteristics over dominant vegetation types in Northeast China, two observational stations were established in Heilongjiang province by the Institute of Atmospheric Environment, China Meteorological Administration in 2012 and 2014, respectively, one in a rice paddy field in Fujin (129.2661°E, 48.2991°N, and 59 m above sea level) and the other one in a mixed forest region in Wuying (131.9385°E, 47.1519°N, and 345 m above sea level) (Figure 1b). The Fujin site was located in the Sanjiang Plain, which has the largest rice production farming region in China (Jia et al., 2018). The Wuying site was located at a national forest park, which remains the largest and well-conserved primitive temperate broad-leaved Korean pine forest in the world (Jia et al., 2018).

#### 2.1.2. Site Observations

EC systems are mounted on a tower at Fujin and Wuying stations to measure turbulence fluctuations of CO<sub>2</sub> concentration, wind speed, and air temperature above the plant canopy with a frequency of 10 Hz. The EC system consists of an open-path CO<sub>2</sub>/H<sub>2</sub>O analyzer (LI-7500, Li-Cor, Inc., USA), a three-dimensional sonic anemometer (CSAT3, Campbell Scientific, Inc., USA), and a data logger (A755GSM-GPRS, Adcon Telemetry, Germany). The observational height is 3.5 and 40 m above ground level (AGL) at Fujin and Wuying sites, respectively. The EC measurements used in this study were taken in 2016, when data continuity was high. The representativeness of the two stations were evaluated using

a footprint analysis method of CO<sub>2</sub> fluxes following Guan et al. (2006). The results showed that approximately 90% of the measured scalar fluxes originated from within 185 and 247 m of the tower at Fujin and Wuying stations, respectively.

In addition, photosynthetically active radiation (PAR) (PAR1, Adcon Telemetry, Germany) is observed at 3.5 m AGL at the Fujin station every 10 min. The PAR data were averaged hourly and then were used to evaluate WRF-VPRM, which employs downwelling shortwave radiation in its parameterization for GEE.

### 2.1.3. Data Processing

We used the turbulent measurement data to calculate friction velocity ( $u_*$ ) and NEE in a 30-min interval (Mauder et al., 2008):

$$u_* = \sqrt[4]{(-\overline{u'w'})^2 + (-\overline{v'w'})^2}, \quad (1)$$

$$NEE = \overline{c'w'}, \quad (2)$$

where  $u'$ ,  $v'$  and  $w'$  are the fluctuations of wind speed in meridional, zonal, and vertical directions, respectively;  $c'$  is the fluctuation of CO<sub>2</sub> concentration.

We followed the quality control method reported by Li et al. (2016) to process the NEE observations. First, we deleted outliers and data with weak turbulence, which often occurs during nighttime and can be distinguished using  $u_* < u_{*c}$ , where  $u_{*c}$  was determined using the method from Zhu et al. (2006) as 0.16 m/s at the rice paddy station (Fujin) and as 0.22 m/s at the mixed forest station (Wuying), respectively. Here, the  $u_{*c}$  at Fujin was higher than that estimated at a rice paddy site (0.10 m/s) during 2015 in Panjin, Liaoning province (Li et al., 2018), and the  $u_{*c}$  at Wuying was close to that used at a forest site (0.20 m/s) in Changbai Mountain from August 2002 to November 2003 (Guan et al., 2006, following Foken & Wichura, 1996). We filled the nighttime gaps based on the fitting equations between the filtered EC-measured NEE and air temperature at night (Li et al., 2016; Zhu et al., 2006). The proportion of filled data to all nighttime data reached about 19.7% at Fujin and 56.4% at Wuying. To avoid the possible impact of filling data on changing the diurnal variation of NEE, the filtered-unfilled data were used for the diurnal variation analysis in this study. For other analysis, the filtered-filled data were used.

## 2.2. Satellite Observations

### 2.2.1. OCO-2 Satellite Observations

We used the OCO-2 Version 9 XCO<sub>2</sub> data retrieved from full physics retrieval as detailed in Kiel et al. (2019) to investigate XCO<sub>2</sub> over Northeast China in 2016. The OCO-2 satellite, launched in 2014, collects data in a Sun-synchronous orbit with a local equator overpass time of 1:30 pm. It measures the intensity of reflected sunlight in three wavelength bands (0.76, 1.60, and 2.06 μm), which are used to infer column average dry air mole fractions of CO<sub>2</sub> (typically denoted by XCO<sub>2</sub>). In this study, we selected a total of 829 XCO<sub>2</sub> samples (quality flag = 0, representing observations without contamination by clouds) over Northeast China at 12:00 Beijing Time (BT), 13:00 local solar time, throughout 2016 for analyzing the monthly variation of XCO<sub>2</sub> in this region and evaluating that simulated by WRF-VPRM.

### 2.2.2. MODIS Satellite Observations

The Enhanced Vegetation Index (EVI), which is closely related to the photosynthetic activity, is a major input for the VPRM (Ahmadov et al., 2007). EVI is responsive to canopy structure variations, including leaf area index, canopy type, plant physiognomy, and canopy architecture (Gao et al., 2000). In this study, EVI was calculated from the MOD09A1 C6 500 m 8-day land surface reflectance data set, retrieved from the MODIS satellite (Huete et al., 2002; Zhang et al., 2017b). Figure 1c shows the distribution of summertime averaged EVI in Northeast China in 2016.

In addition, land use types (referred to as plant functional types in Hilton et al., 2013) used in WRF-VPRM to calculate CO<sub>2</sub> fluxes, currently classified into seven categories, namely, evergreen forest, deciduous forest, mixed forest, shrubland, savannah, cropland, and grassland, are also derived from MODIS land cover product (MOD12Q1) (Zhang et al., 2017b).

**Table 1**  
The VPRM Parameter Values Over Seven Vegetation Types Used in This Study

	Crops	Mixed forest	Evergreen forest	Deciduous forest	Shrub	Savanna	Grass
$\alpha$	0.1300	0.2000	0.1247	0.0920	0.0634	0.2000	0.0515
$\beta$	0.5420	0.27248	0.2496	0.8430	0.2684	0.3376	-0.0986
$\lambda$	0.085	0.100	0.130	0.100	0.180	0.180	0.115
$PAR_0$	1074.9	419.50	745.306	514.13	590.7	600.0	717.1

Note. Units are as follows:  $\alpha$ ,  $\mu\text{mol CO}_2\text{-m}^{-2}\text{-s}^{-1}$ ;  $\beta$ ,  $\mu\text{mol CO}_2\text{-m}^{-2}\text{-s}^{-1}$ ;  $\lambda$ ,  $\mu\text{mol CO}_2\text{-m}^{-2}\text{-s}^{-1}/\mu\text{mol PAR}\text{-m}^{-2}\text{-s}^{-1}$ ; and  $PAR_0$ ,  $\mu\text{mol PAR}\text{-m}^{-2}\text{-s}^{-1}$ .

### 2.3. Online Coupled Weather-Biosphere Modeling

#### 2.3.1. WRF-VPRM

VPRM is fully coupled with the WRF model that considers impact of WRF-simulated meteorological fields on calculation of terrestrial  $\text{CO}_2$  fluxes every time step and computes transport of  $\text{CO}_2$  using simulated continuous meteorological fields (Ahmadov et al., 2007). VPRM simulates NEE as the sum of ecosystem respiration (ER) and GEE (Mahadevan et al., 2008):

$$NEE = ER + GEE. \quad (3)$$

NEE and GEE are defined as the net and gross  $\text{CO}_2$  fluxes between the ecosystem and the atmosphere, respectively. ER is  $\text{CO}_2$  flux caused by respiration of all organisms, including autotrophic respiration  $ER_a$  (caused by vegetation) and heterotrophic respiration  $ER_h$  (caused by symbiotic microorganisms in soil). These definitions are based on the view of micrometeorology and take the atmosphere as a reference to determine the flux sign. Flux to the atmosphere increases atmospheric  $\text{CO}_2$  mole fraction and is defined to be positive. GEE represents those fluxes caused by plant photosynthesis and thus always has a negative sign, while ER always has a positive sign. NEE and GEE are equivalent to net ecosystem production and gross primary production (GPP) except that Net Ecosystem Production and GPP take the ecosystem as a reference and they have an opposite sign (Chapin et al., 2005). Hereafter, we will only use NEE and GEE. ER and GEE in VPRM are parameterized as

$$ER = (\alpha \times T) + \beta, \quad (4)$$

$$GEE = -\lambda \times T_{scale} \times W_{scale} \times P_{scale} \times \frac{1}{1 + \frac{PAR}{PAR_0}} \times FAPAR_{PAV} \times PAR, \quad (5)$$

where  $T$  is the air temperature at 2 m AGL ( $T_a$ ) in WRF-VPRM simulation and  $\alpha$  and  $\beta$  are two empirical parameters. When  $T < -\beta/\alpha$ , ER is set to zero. GEE depends on more variables, including the maximum LUE  $\lambda$ , temperature scale  $T_{scale}$ , water stress scale  $W_{scale}$ , phenology scale  $P_{scale}$ , PAR, its half-saturation value  $PAR_0$ , and the fraction of PAR absorbed by the photosynthetically active portion of the vegetation ( $FAPAR_{PAV}$ ). The  $FAPAR_{PAV}$  is proportional to EVI, and here we set  $FAPAR_{PAV}$  equal to the MODIS 8-day-updated EVI according to Mahadevan et al. (2008). PAR is calculated using the shortwave (SW) downward radiation as  $SW/0.505$  (Mahadevan et al., 2008). The values of four empirical parameters ( $\alpha$ ,  $\beta$ ,  $\lambda$ , and  $PAR_0$ ) for seven land use categories used in this study (summarized in Table 1) were calibrated previously by Hilton et al. (2013) using data from 65 EC towers over North America. Note that the calibrated parameters varied between different towers among the same land use category over the North America, and we used the median values from different towers in each category for all the seven categories. The variation of optimal parameters at different locations over the same MODIS-derived land use category may be even larger if they are also calibrated outside of North America, including Northeast China, because the specific soil and plants that fall into each category vary across continents.

#### 2.3.2. Model Setup

Table 2 summarizes the model configurations. WRF-VPRM is configured with two domains including China and nested Northeast China domain (Figure 1a) with a horizontal resolution of 20 and 4 km, respectively. Both model domains have 47 vertical layers extending from the surface to 10 hPa. The simulations ran

**Table 2**  
*WRF-VPRM Model Configurations*

Reference	Attribute	Model configuration
Dudhia (1989)	Short wave radiation	Dudhia algorithm
Mlawer et al. (1997)	Long wave radiation	Rapid radiative transfer model (RRTM)
Hong et al. (2006)	Boundary layer	Yonsei University (YSU) scheme
Morrison et al. (2009)	Microphysics	Morrison microphysics scheme
Chen and Dudhia (2001)	Land surface model	Noah land-surface scheme
Wang and Kotamarthi (2014)	Cumulus	Grell-Freitas scheme
	Interior nudging	Spectral nudging
	Nudging variables	Horizontal wind components, temperature, geopotential
	Nudging coefficient	$3 \times 10^{-5} \text{ s}^{-1}$
	Nudging height	Above PBL
	Wave number	5 and 3 in the zonal and meridional directions respectively

continuously from 1 January to 31 December 2016 using spectral nudging and climatic downscaling techniques documented by Hu et al. (2017, 2018, 2019b) and Li et al. (2019). Temperature, geopotential height, and horizontal winds above the boundary layer at a  $\sim 1,000$  km scale are spectrally nudged to the reanalysis data throughout the downscaling simulation, and variation of these variables over smaller scales are predicted by model dynamics.  $T_a$  used to drive VPRM is not directly simulated but diagnosed from temperature at the land surface and the lowest model layers (Hu et al., 2010a), none of which are nudged to the reanalysis data.

The National Center for Environmental Prediction/DOE R2 data (Kanamitsu et al., 2002) provide the meteorological initial and boundary conditions, and the  $3^\circ \times 2^\circ$  global CarbonTracker model outputs (version CT2017, released in 2018) provide atmospheric  $\text{CO}_2$  initial and boundary conditions (Peters et al., 2007, with updates at <https://www.esrl.noaa.gov/gmd/ccgg/carbontracker/>). The CT2017 system assimilates in situ  $\text{CO}_2$  observations around the world to produce the optimal estimation of global  $\text{CO}_2$  fields (CarbonTracker Team, 2018). The CT2017  $\text{CO}_2$  fields have been evaluated and validated by Yuan et al. (2019) and Bernath et al. (2019). The simulations also include anthropogenic and oceanic  $\text{CO}_2$  emissions. The  $0.1^\circ \times 0.1^\circ$  Open-source Data Inventory for Anthropogenic  $\text{CO}_2$  data set provides the monthly anthropogenic emissions of  $\text{CO}_2$ , as recommended by Hu et al. (2019a). The monthly ocean  $\text{CO}_2$  fluxes are from a  $4^\circ \times 5^\circ$  global ocean climatological database, which includes more than 3 million partial pressure  $\text{CO}_2$  measurements (Takahashi et al., 2009). The  $0.1^\circ \times 0.1^\circ$  and  $4^\circ \times 5^\circ$  emission data are mapped to the modeling domain with a grid spacing of 4 km through spatial interpolation, following a common practice for most simulations with the WRF model with chemistry (WRF-Chem) (Hu et al., 2013, 2014, 2019a; Thomas et al., 2019).

#### 2.4. Parametric Uncertainty Analysis Using Off-Line VPRM

There are reducible and irreducible uncertainties in WRF-VPRM  $\text{CO}_2$  simulations. The irreducible uncertainties are attributable to the challenge of accurately quantifying the stochastic variations in atmospheric dynamics (Gilliam et al., 2015; Zhang et al., 2016). The reducible uncertainties are caused by model errors (including the structure error and parametric uncertainties) and biases in model input data (including initial and boundary conditions, as well as emissions). Analyzing reducible uncertainties can assess the accuracy and practical predictability of  $\text{CO}_2$  fields and further improve the model performance.

In this study, we focused on examining the parametric uncertainties of VPRM in relation to  $\alpha$ ,  $\beta$ ,  $\lambda$ , and  $\text{PAR}_0$ , which has a larger impact on the uncertainties in simulated NEE than other variables and parameters used in VPRM (to be discussed in sections 3.1 and 3.5). Since  $\text{CO}_2$  does not affect the meteorological variables in the simulations, we examined parameter sensitivities using off-line VPRM simulations with meteorology from the standard WRF-VPRM run and focused on the impact of parametric uncertainties on simulated  $\text{CO}_2$  fluxes. In the sensitivity studies, five ensemble simulations (one multiparameter experiment and four single-parameter experiments) were designed following the methods in Nielsen-Gammon et al. (2010), in which the model input parameters were randomly perturbed within reasonable ranges to examine the sensitivity of model outputs to different parameter values. In the multiparameter experiment, we randomly perturbed four parameters simultaneously to examine the uncertainties of NEE simulations due to their

**Table 3**  
Range of VPRM Parameters in Five Groups of Ensemble Simulations

Ensemble simulation	$\alpha$	$\beta$	$\lambda$	PAR <sub>0</sub>
ES1	[0.12, 0.30]	[0.50, 1.20]	[0.09, 0.14]	[350, 600]
ES2	[0.12, 0.30]	1	0.1	419.5
ES3	0.2	[0.50, 1.20]	0.1	419.5
ES4	0.2	1	[0.09, 0.14]	419.5
ES5	0.2	1	0.1	[350, 600]

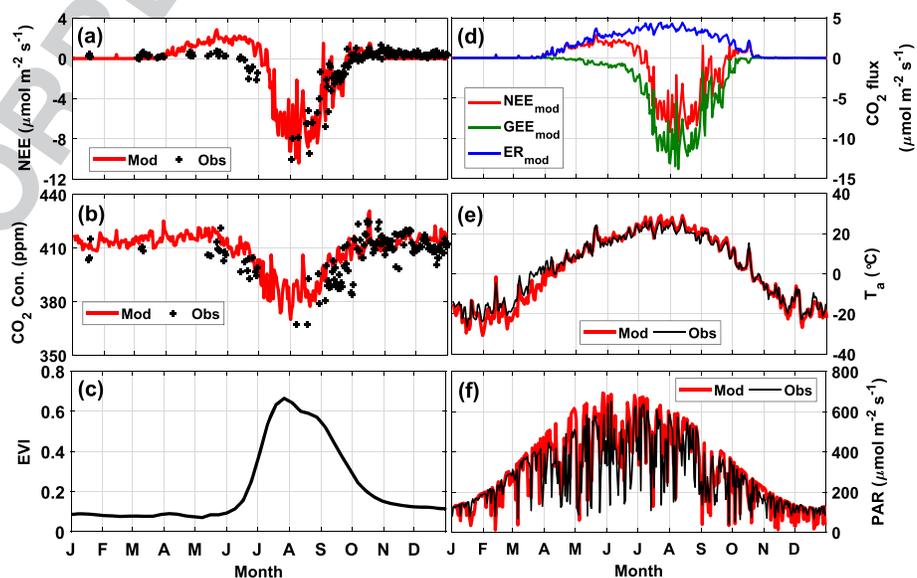
parametric uncertainties, while in each single-parameter experiment, we only perturbed one parameter and kept other parameters unchanged to isolate the sensitivities of model outputs due to a single parameter. Similar ensemble simulations have been widely used to analyze uncertainties and predictability in atmospheric chemical transport models in previous studies (e.g., Gneiting & Raftery, 2005; Hu et al., 2010b; Krishnamurti et al., 2000; Nielsen-Gammon et al., 2010; Pinder et al., 2008; Zhang et al., 2007).

In these ensemble simulations, we randomly generated 100 values from a reasonable range for each parameter (see Table 3). The relative range of each VPRM parameter was  $-40\%$ – $50\%$  for  $\alpha$ ,  $-50\%$ – $20\%$  for  $\beta$ ,  $-10\%$ – $40\%$  for  $\lambda$ , and  $-16.57\%$ – $43.03\%$  for PAR<sub>0</sub>. The variation ranges were located within those obtained at 65 EC sites in North American (see Figure 3 in Hilton et al., 2013) and can likely cover the uncertainties of NEE at the mixed forest station. Second, we ran the multiparameter ensemble simulation (ES1) using the 100 combinations of the four VPRM parameters to calculate the NEE, that is,  $NEE_{ES1}(i,t) = f\{\alpha(i),\beta(i),\lambda(i),PAR_0(i),t\}$ , with  $i = 1, 2, \dots, 100$  and  $t$  being the time (different hours in the growing season). In the single-parameter ensemble simulations, ES2, ES3, ES4, and ES5, we ran off-line VPRM using 100 values of one parameter but keeping the other three fixed at the original value (see Table 3). All five experiments were conducted under the growing season of 2016 at the mixed forest station, driven by the WRF-simulated  $T_a$  and PAR. Finally, we compared the mean diurnal variation of NEE during the growing season (in terms of the variation range, the mean value, and standard deviation) from ES1–ES5 with the observations and online WRF-VPRM simulation. We also calculated the differences of the growing-season-averaged NEE between each member in ES1–ES5 and WRF-VPRM and attributed these differences to the relative variation ratios of each VPRM parameter.

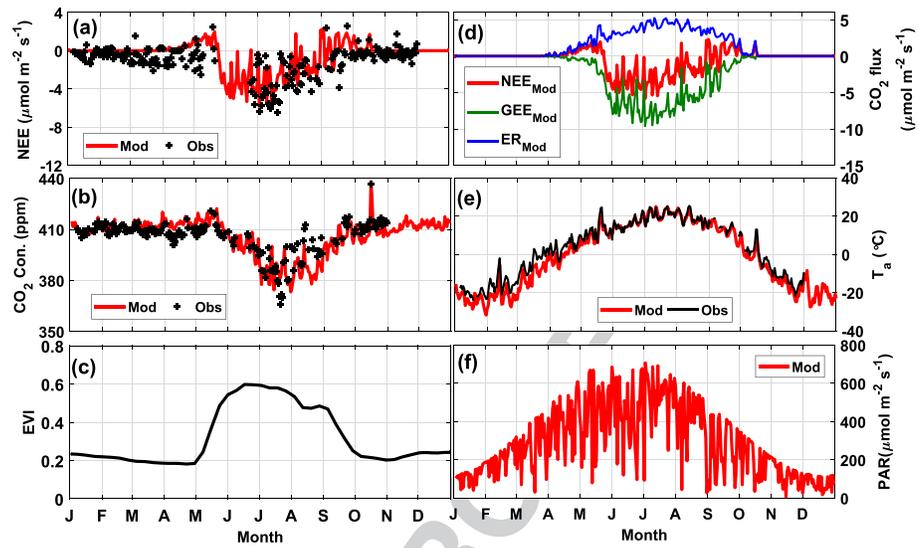
### 3. Results

#### 3.1. Seasonal Variations of the NEE and Surface CO<sub>2</sub> Concentrations

Seasonal variations of the NEE and surface CO<sub>2</sub> concentrations at Fujin (rice paddy) and Wuying (mixed forest) stations are first examined (Figures 3a, 3b, 4a, and 4b). At Fujin station, negative daily mean NEEs were observed from mid-June to the end of September. The minimum daily mean NEE of  $-10 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$



**Figure 3.** Temporal variations of daily mean observed and simulated (a) net ecosystem exchange (NEE) and (b) surface concentration of CO<sub>2</sub>, (c) enhanced vegetation index (EVI) linearly interpolated based on MODIS 8-day-update EVI, (d) simulated NEE, gross ecosystem exchange (GEE), and respiration term (ER), observed and simulated (e) air temperature, and (f) photosynthetically active radiation (PAR) at the rice paddy site in Fujin during 2016.



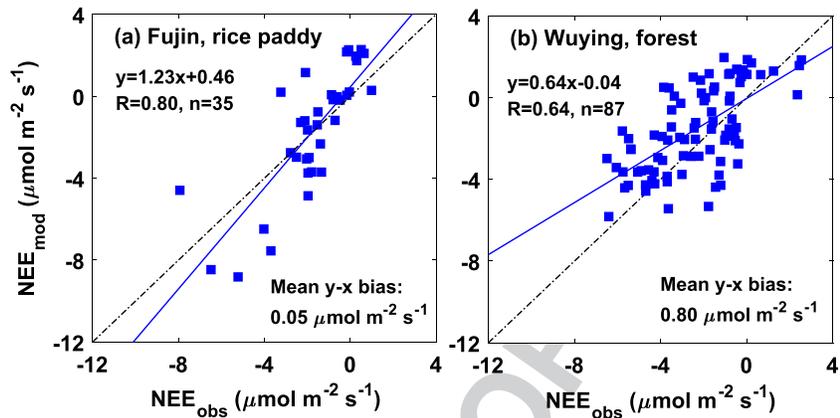
**Figure 4.** The same as Figure 3 but for the mixed forest site in Wuying without observations of photosynthetically active radiation (PAR).

occurred in the early August. In the nongrowing season, the daily mean NEE mostly exhibited low positive values ( $<1.5 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) (Figure 3a). At Wuying station, the NEE started decreasing in mid-May, 1 month earlier than that observed at Fujin, and reached the minimum value of  $-6.5 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  in July. After reaching the minimum, the NEE increased gradually till the end of September and then varied between  $\pm 2.5 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  in the rest time period (Figure 4a). The seasonal variations of NEE and surface  $\text{CO}_2$  concentrations at both stations were primarily controlled by EVI (Figures 3c and 4c). With the increase of EVI in summer, the uptake of  $\text{CO}_2$  increased due to enhanced ecosystem photosynthesis, resulting in lower surface  $\text{CO}_2$  concentrations in summer compared to in other seasons at both stations (Figures 3b and 4b).

These results are consistent with previous studies. For example, the seasonal variation of NEE at Fujin was consistent with that observed at a rice paddy site ( $41^{\circ}11'N$ ,  $121^{\circ}54'E$ ) in Liaohe Plain during 2005 (Li et al., 2018) and a rice paddy site ( $47^{\circ}35'N$ ,  $133^{\circ}31'E$ ) in Sanjiang Plain during 2004 (Song et al., 2006). Both previous works showed the NEE decreased after mid-June and reached the lowest value in late-July. The observed daily mean NEE in Song et al. (2006) ranged from  $-13$  to  $4 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ , which is slightly wider than the range observed at Fujin, though for a different year. The seasonal variation of NEE observed at Wuying was close to the observations at a mixed forest station ( $42^{\circ}24'09"N$ ,  $128^{\circ}05'45"E$ , 738 m) in the Changbai Mountains during 2003 (Guan et al., 2006), in which the daily mean NEE decreased since May and reached the lowest value in late June, ranging from  $-6.5$  to  $2.0 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  throughout the year.

WRF-VPRM successfully captured the seasonal variations of NEE and surface  $\text{CO}_2$  concentrations at both stations and performed especially well at Fujin (Figures 3a, 3b, 4a, and 4b). During the growing season, the simulated daily mean NEE was similar to the observations at Fujin, with a correlation coefficient ( $R$ ) of 0.80 and a mean bias of  $0.05 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ , and at Wuying, with a  $R$  of 0.64 and a mean bias of  $0.80 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  (Figure 5). Although the model reproduced NEE at Fujin well in other time periods, it overestimated NEE from April to June. To diagnose the NEE bias, we examined the simulated GEE, ER, and driving meteorological variables including  $T_a$  and PAR (Figures 3d–3f and 4d–4f).

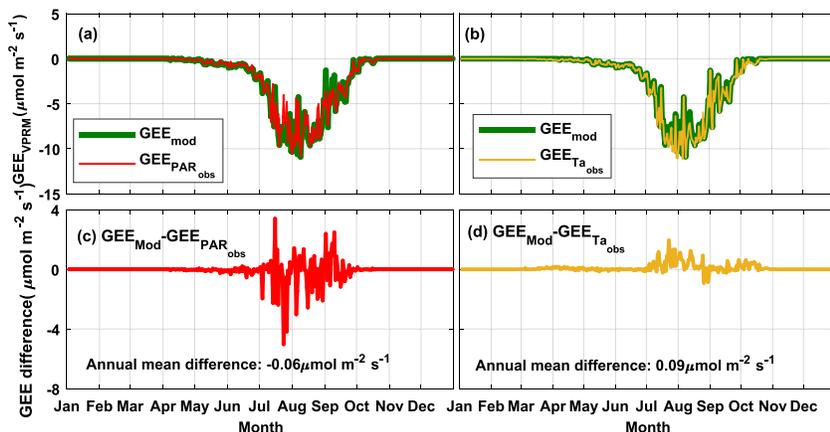
The WRF model reproduced the daily variations of  $T_a$  throughout the year well, with a  $R$  of  $\geq 0.98$  between the simulated and observed  $T_a$  at both stations. Simulated and observed PAR at Fujin had a  $R$  of 0.87. From April to August, PAR at Fujin was overestimated by  $78 \text{ W/m}^2$  on average. To isolate the impact of biases of individual meteorological variables (i.e., PAR and  $T_a$ ) on simulated GEE and NEE, off-line VPRM simulations were conducted with both simulated and observed meteorological variables at the Fujin station throughout 2016 (Figure 6). These off-line VPRM simulations indicated that the biases of PAR had a greater impact on GEE simulations on individual days than the biases of  $T_a$ . The uncertainties of simulated GEE caused by the biases of PAR ranged from  $-5.0$  to  $3.4 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ , while the uncertainties caused by the



**Figure 5.** Relationships between observed and simulated daily mean NEE during the growing seasons (from May to September, only on days with observational rate >90%) at (a) the Fujin rice paddy site and (b) the Wuying mixed forest sites. Black line represents the 1:1 line, and blue line represents the fitting equation.

biases of  $T_a$  varied between  $-0.9$  and  $2.0 \mu\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$  throughout 2016 at Fujin on individual days. On seasonal or annual scales, the impacts on simulating GEE by PAR or  $T_a$  biases were negligible. The biases of PAR and  $T_a$  contributed a mean uncertainty of simulated GEE of  $-0.17$  and  $0.16 \mu\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$  during the growing season and of  $-0.06$  and  $0.09 \mu\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$  during the entire year, which was much smaller than that caused by the uncertainties in the four VPRM parameters (reaching  $-4 \mu\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$  averaged in the growing season at the most and to be discussed in section 3.5).

In addition to biases in meteorological variables, the NEE modeling bias is also generated from the model errors associated with VPRM itself. Examination of GEE and ER at Fujin station indicates the NEE bias from April to June may be dominantly due to model bias of ER. During April to June, the simulated GEE remained near zero because of low EVI, and meanwhile, the simulated ER increased with the increasing  $T_a$  (above  $0^\circ \text{C}$  approximately). In VPRM, while the GEE depends on more variables and is largely dictated by EVI, the ER only linearly depends on  $T_a$ . In addition to the linear function used in VPRM, an exponential function between ER and  $T_a$  has been suggested to simulate ER (Fang & Moncrieff, 2001; Lloyd & Taylor, 1994). With an exponential parameterization, the increase of ER with  $T_a$  becomes relatively slow when  $T_a$  is small and gradually enhances with the increase of  $T_a$  (Figure S1 in the supporting information). Thus, adopting the exponential parameterization might help to alleviate the bias of simulated ER at least over the rice paddy, particularly in spring with low EVI and increasing  $T_a$ . It could also probably produce



**Figure 6.** Simulated GEE driven by simulated and observed (a) PAR and (b)  $T_a$  and (c and d) the corresponding difference of simulated GEE driven by simulated and observed values.

better results of simulating ER to parameterize plant respiration (which is part of ER) with EVI as well as temperature, since ER depends not only on temperature but also on the mass of leaf and stem of biomes that can be roughly represented by EVI (Guan et al., 2006). The leaf and stem respiration was observed to account for about 27% of the total ER in an old-growth forest area in the Great Lakes region of the United States during 2002 and 2003 on average (Tang et al., 2008). A higher proportion (about 52%) was estimated in a temperate mixed forest area in Northeast China (Guan et al., 2006). Therefore, when the EVI was low at Fujin rice station, the values of ER should increase more slowly with  $T_a$  due to the limited leaf and stem respiration. These structural deficiency of the VPRM in simulating ER (linear dependency on  $T_a$  and not considering EVI) ultimately resulted in an overestimation of NEE at Fujin from April to June. Similar phenomenon also occurred in May at Wuying, but to a less extent.

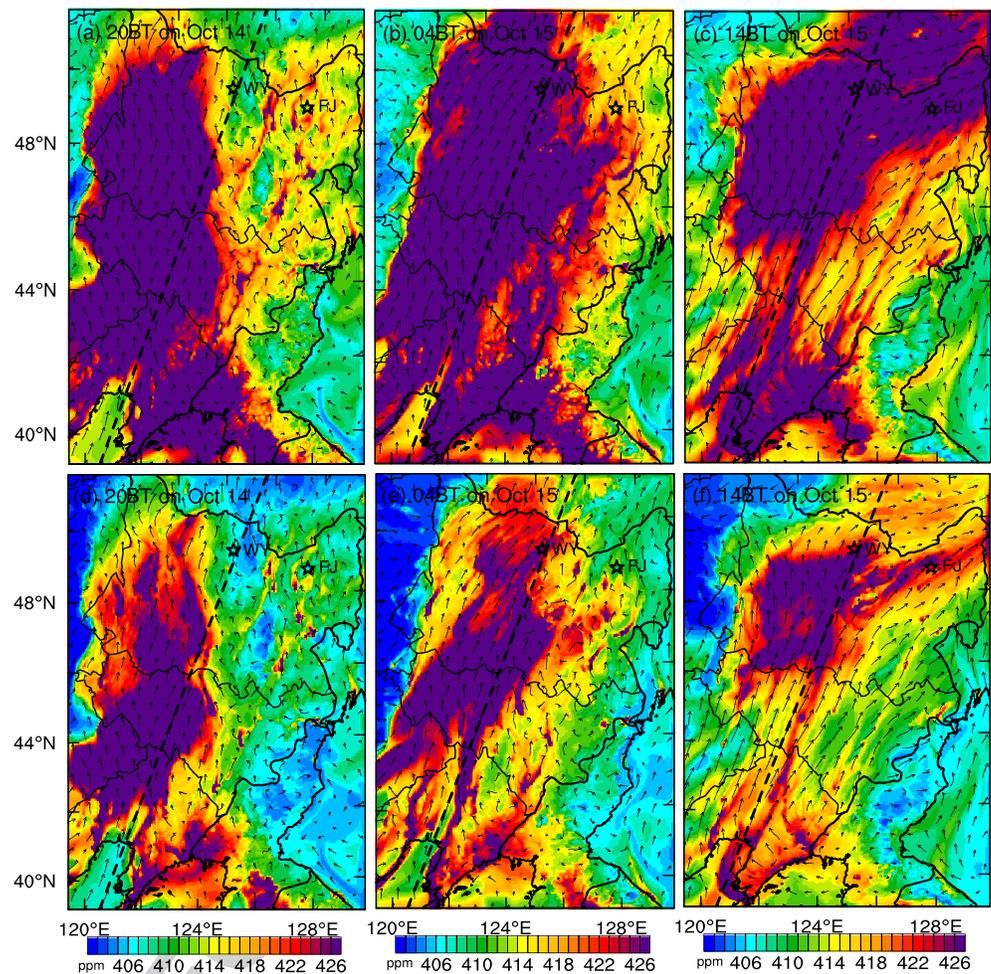
Setting ER as zero when  $T_a \leq -\beta/\alpha$  in current VPRM is another error source in cold seasons (from October to April in Northeast China). Many existing observational studies illustrated that total ER remained above zero in cold seasons. For example, Tang et al. (2008) observed that the wintertime daily mean ER remained about  $1 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  in an old-growth forest area in the Great Lakes region of the United States. Ren et al. (2007) reported that the hourly mean soil respiration ranged from 0.3 to  $2.5 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  during the nongrowing season in a paddy ecosystem in the subtropical region of China. Mahadevan et al. (2008) adopted different  $T_{\text{low}}$ , with the  $T_{\text{low}}$  varying from 1 to 5 °C, for different vegetation types, to calculate ER replacing  $T_a$  in presence of  $T_a < T_{\text{low}}$  for optimal VPRM simulation. We examined the potential optimal  $T_{\text{low}}$  for VPRM simulation over Fujin. Off-line VPRM simulations were conducted with different  $T_{\text{low}}$  values (0, 1, 2, and 5 °C) at the Fujin station (Figure S2). Simulated daily mean ER increased by  $0.1 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  approximately with an increase of 1 °C in  $T_{\text{low}}$  from January to March and from November to December. During the two periods, setting  $T_{\text{low}}$  as 0 °C could obtain a mean ER value ( $0.50 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) closer to the observed one ( $0.42 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ). During warm season, the simulated ER did not depend on  $T_{\text{low}}$  at most time. In sum, the ER error in cold season is likely due to the VPRM structure errors, which can be reduced by modeling biogenic respiration with more realism.

The uncertainties associated with the VPRM parameters may introduce model bias of GEE. The VPRM parameters for the seven land use categories used in this study were calibrated using data from 65 EC towers over North America. These calibrated parameters even varied among different towers for the same land use category in North America (Hilton et al., 2013); the optimal VPRM parameters over each individual land use category may also vary from North America to Northeast China due to different soil and plants (Diao et al., 2015), even though the same land surface may be chosen using MODIS data. Limited work has been done to optimize the VPRM parameters in China. For example, Liu et al. (2015) and Zhang et al. (Zhang et al., 2017a) optimized the VPRM parameters at a subtropical evergreen forest site and a mixed forest site in Changbai Mountains, respectively, and the NEE simulations are improved using the optimized VPRM parameters. Dayalu et al. (2018) calibrated the four VPRM parameters for different vegetation types using EC measurements at six stations in China. However, these calibrated VPRM parameters in China have large uncertainties. The uncertainty of simulated NEE due to VPRM parameters will be discussed in section 3.5.

Finally, the biases of simulated GEE in WRF-VPRM may also come from the uncertainty of simple parameterization of GEE as a function of satellite-derived variables, for example, EVI, which may not be a true indicator of total biomass (Matsushita et al., 2007; Shi et al., 2017). In theory, calculating GEE using more accurate estimation of total biomass in process-based models may be more accurate, given that all the involved parameters are carefully calibrated using observations (Farquhar et al., 1980; Pury & Farquhar, 1997; White et al., 2000). However, in most cases, observations are insufficient to calibrate the parameters in more detailed process-based models using more accurate biomass (White et al., 2000), particularly over observation-sparse regions like China. LUE models such as VPRM, even though parameterizing GEE using a crude function of EVI, provide a good compromise between applicability and process details in three-dimensional simulations (Zhang et al., 2017b).

### 3.2. Episodic Variation of NEE and Surface CO<sub>2</sub> Concentrations on 15 October

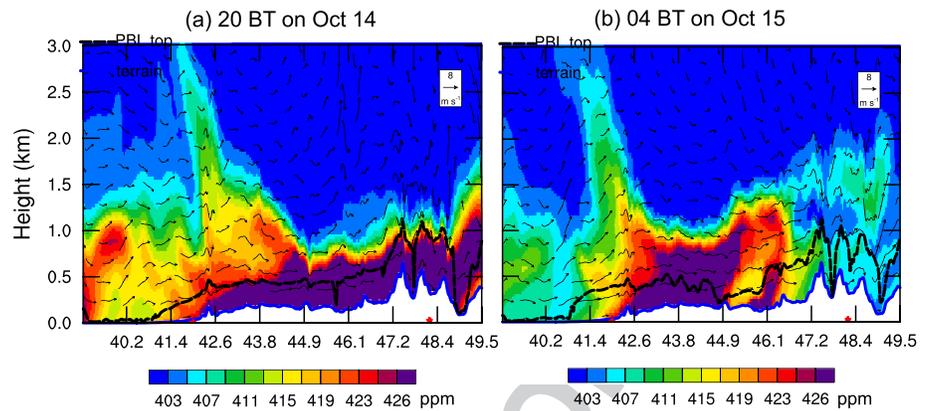
Superimposed on the seasonal variation of NEE and surface CO<sub>2</sub> concentrations, a few episodic variations are prominent, which are due to synoptic weather events, such as frontal passages. The highest CO<sub>2</sub>



**Figure 7.** Spatial distributions of simulated surface CO<sub>2</sub> concentrations (including biogenic and anthropogenic contributions) over Northeast China at (a) 20:00 BT on 14 October, (b) 04:00 BT and (c) 14:00 BT on 15 October 2016, and (d–f) those excluding biogenic contribution. Black stars represent the locations of Wuying (WY) and Fujin (FJ) stations. Arrows represent horizontal wind vectors at 10 m AGL.

concentration throughout 2016 with a distinct spike in NEE appeared on 15 October at both Fujin and Wuying. The WRF-VPRM simulation well reproduced the episodic variations at both stations.

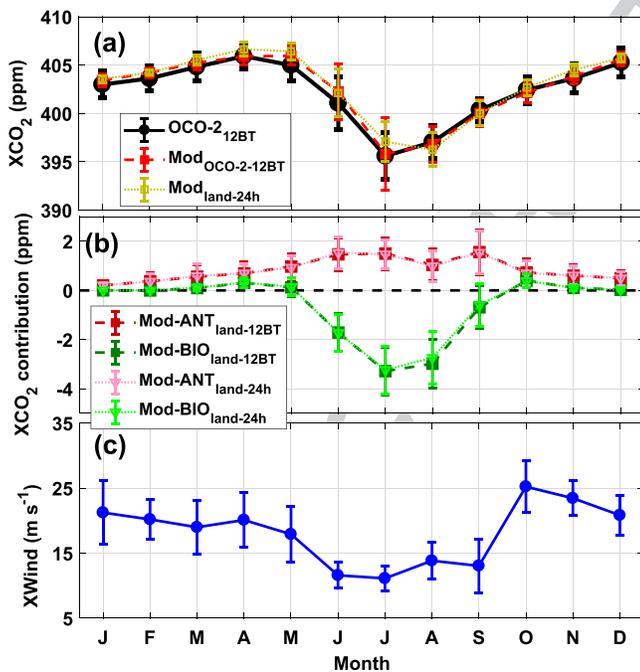
We analyzed causes of the high CO<sub>2</sub> episode on 15 October 15. Figure 7 displays the spatial distributions of surface CO<sub>2</sub> concentrations at different time during this episode in Northeast China. The upper three plots are simulation outputs with both anthropogenic emissions and biogenic fluxes, and the bottom three plots are with anthropogenic emissions only. At 20:00 BT on 14 October (Figure 7a), the CO<sub>2</sub> was concentrated in the southern and western regions of Northeast China, where strong southerly flows dominated; thereafter, wind direction turned from the south to the southwest. As a result, CO<sub>2</sub> moved northeastward arriving at Wuying at 04:00 BT on 15 October (Figure 7b) and then Fujin at 14:00 BT on 15 October (Figure 7c). The low-level southwesterly flows can be accelerated by the upper troposphere East Asian subtropical westerly jet, which covered regions with latitudes higher than 40°N, including Northeast China, through downward momentum transport (Kuang et al., 2007; Uccellini & Johnson, 1979). Moreover, local geography can also contribute to the strong southwesterly flows near the surface. The northward moving airflow can be accelerated and tends to have an increase in its anticyclonic vorticity as the Coriolis parameter increases with increasing latitude because of conservation of potential vorticity (Wexler, 1961; Zhong et al., 1996). This means southerly winds from North China Plain, blocked by the southwest-northeast oriented mountains, can become stronger and veer clockwise when arriving at Northeast China (Figure S3). Besides the



**Figure 8.** Height-latitude cross sections of simulated total CO<sub>2</sub> concentration (including biogenic and anthropogenic contributions) along the dash line in Figure 7 at (a) 20:00 BT on 14 October and (b) 04:00 BT on 15 October 2016. The red star represents the location of Wuying station. Arrows represent wind vectors.

horizontal CO<sub>2</sub> transport, subsiding air flows also favored the CO<sub>2</sub> accumulation near the surface (Figure 8). The CO<sub>2</sub> was accumulated in the air under 1 km (Lat. from ~42.0° to ~47.0°) at 20:00 BT on October 14 (Figure 8a). The depth of CO<sub>2</sub>-rich layer decreased over time due to strong subsidence between 41–47°N (Figure S4), facilitating farther northeast transport (Figure 8b).

In addition to the favorable meteorological conditions, ER played a significant role in enhancing CO<sub>2</sub> in this episode due to an increase of 7 °C in  $T_a$  (see in Figures 3e and 4e). On 15 October, Northeast China was located ahead of a transverse trough, and strong warm advection at low altitudes (at 925 and 850 hPa) favored to the abrupt increase in  $T_a$  in this region. Without biogenic fluxes, the simulated surface CO<sub>2</sub> concentrations decreased significantly in most region of Northeast China, including Wuying and Fujin (Figures 7d–7f). During this episode, the anthropogenic and biotic fluxes each contributed about  $59.4 \pm 5.9\%$  and  $40.6 \pm 5.9\%$  to the increase of surface CO<sub>2</sub> concentrations at Wuying.



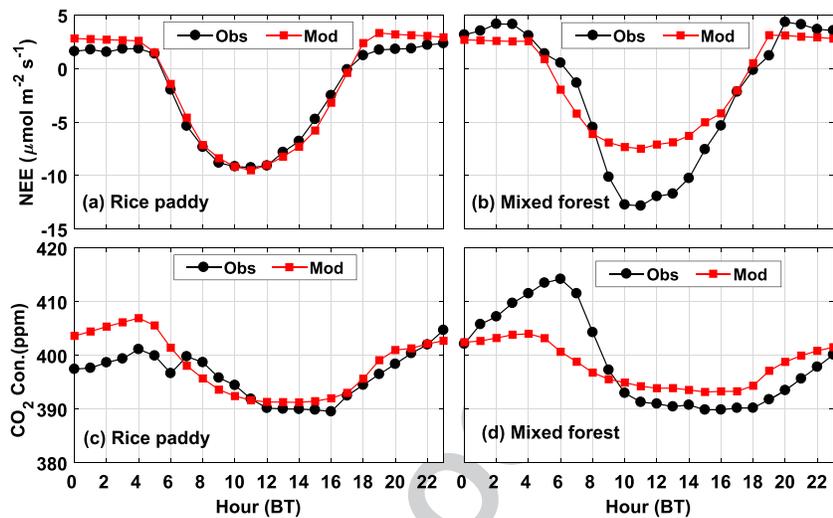
**Figure 9.** Monthly variations of (a) OCO-2-retrieved 12:00 BT XCO<sub>2</sub> (black), correspondingly simulated XCO<sub>2</sub> (red), and 24-hr land-surface averaged XCO<sub>2</sub> (yellow); (b) the simulated 12:00 BT (red) and 24-hr (green) land-surface averaged biogenic and anthropogenic contributions of XCO<sub>2</sub>; and (c) the simulated 12:00 BT land-surface averaged column-averaged wind speed in Northeast China during 2016. Error bars represent standard deviation.

### 3.3. Source Contributions to XCO<sub>2</sub>

Radiative/climate forcing is exerted by greenhouse gases in the whole column of the atmosphere, rather than only from the surface. Thus, in addition to near-surface variables, we also examined the total column abundance of CO<sub>2</sub> (XCO<sub>2</sub>). We first compare simulations with the OCO-2-retrieved XCO<sub>2</sub> data set to evaluate the performance of WRF-VPRM and then use the model simulations to assess the biogenic and anthropogenic contributions to XCO<sub>2</sub> in Northeast China.

#### 3.3.1. Seasonal Variation of XCO<sub>2</sub>

The monthly variation of mean XCO<sub>2</sub> in 2016 over Northeast China was evaluated using data from the OCO-2 satellite (Figure 9a) that has a local overpass time of 1:30 PM (12:30 BT). The simulated XCO<sub>2</sub> at 12:00 BT varied consistently with the OCO-2-retrieved XCO<sub>2</sub>, with an averaged bias of  $0.29 \pm 0.48$  ppm; both showed the lowest value in July (summer) and the highest value in April (spring). The monthly variation range of both observed and simulated XCO<sub>2</sub> over Northeast China was approximately 10 ppm in 2016 in this study. A slightly larger month variation of XCO<sub>2</sub> (>11 ppm) over the same region was reported by Yang et al. (2016) for 2010 based on the measurements of the Greenhouse gases Observing SATellite. Such a seasonal variation is stronger than that in other regions in China (Xu et al., 2017; Yang et al., 2016). The larger seasonal variation



**Figure 10.** Mean diurnal variations of the observed and simulated (a and b) NEE and (c and d) surface CO<sub>2</sub> concentrations at Fujin rice paddy station and at Wuying mixed forest station during the growing season (May through September) in 2016.

of XCO<sub>2</sub> in Northeast China is caused by significant terrestrial CO<sub>2</sub> fluxes in the region (Yang et al., 2016) and enhanced north-to-south XCO<sub>2</sub> gradient on a larger scale in North Hemisphere in summer (Yang et al., 2018).

### 3.3.2. Anthropogenic and Biogenic Contributions to XCO<sub>2</sub>

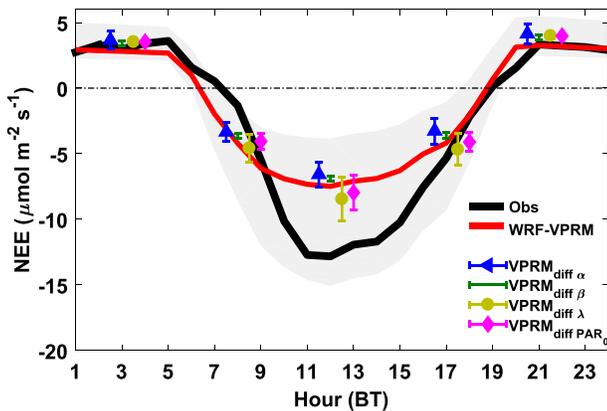
Using the WRF-VPRM simulation, we estimated the monthly contributions to XCO<sub>2</sub> from different sources, including anthropogenic emissions and biogenic and oceanic fluxes, averaged over land surface of Northeast China (Figure 9b). Oceanic contribution from nearby Chinese oceans was negligible, two orders smaller in magnitude than anthropogenic and biogenic contributions, thus is not shown in Figure 9. The monthly mean anthropogenic and biogenic contribution at 12:00 BT and over 24 hr are virtually the same, even for biogenic fluxes that have a prominent diurnal variation in the growing season. While diurnal variation of biogenic flux generally follows diurnal variation of radiation, thus reaching maximum uptake flux during noon time (Figure 10), diurnal variation of its contribution to XCO<sub>2</sub> lags behind by ~5 hr, showing a maximum drawdown of XCO<sub>2</sub> around 17:00 BT during the growing season (Figure S5), similar as previously reported by Olsen and Randerson (2004). As a result of such a diurnal variation, biogenic contribution to XCO<sub>2</sub> at 12:00 BT roughly equals its contribution over the whole day.

Anthropogenic emissions contributed 0.21–1.54 ppm to XCO<sub>2</sub> in each month, with contribution during summer months being three times larger than the annual mean contribution. The seasonal variation of Open-source Data Inventory for Anthropogenic CO<sub>2</sub> anthropogenic emissions averaged in Northeast China was from 0.65 to 0.83 μmol·m<sup>-2</sup>·s<sup>-1</sup> (not shown). During June–September, the mean anthropogenic emission (0.745 μmol·m<sup>-2</sup>·s<sup>-1</sup>) was 2% higher than the annual mean of 0.738 μmol·m<sup>-2</sup>·s<sup>-1</sup>, which cannot explain a threefold increase of anthropogenic contribution of XCO<sub>2</sub> during summer months comparing with the annual mean contribution. Instead, the monthly variation of winds likely dictated the monthly variation of anthropogenic contribution. The column-averaged wind speed (denoted as XWind, computed similarly as XCO<sub>2</sub>) from June to September in Northeast China was observed 32% lower than the annual mean level (Figure 9c). The weak winds in summer favored the accumulation of CO<sub>2</sub> within local areas.

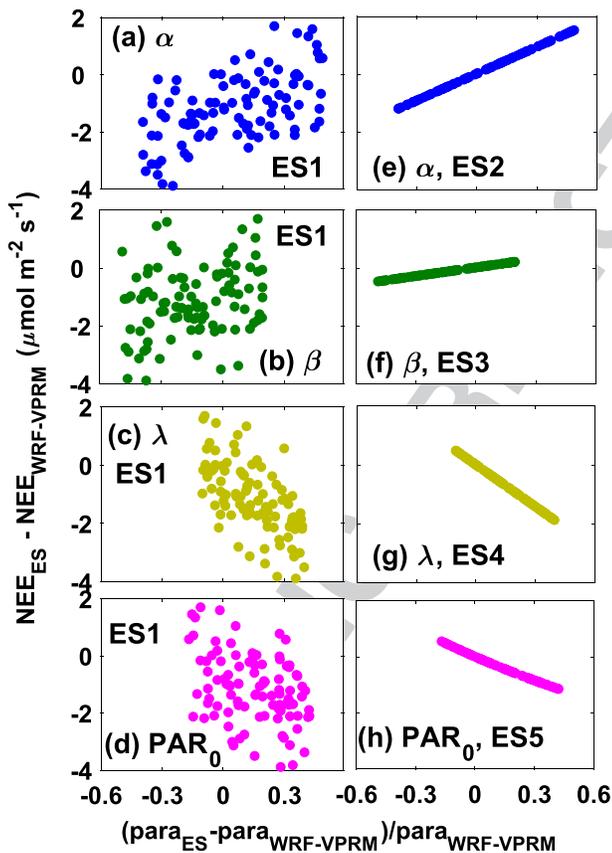
Terrestrial ecosystems acted as a CO<sub>2</sub> sink from June to September in Northeast China, contributing –3.22 to –0.60 ppm to XCO<sub>2</sub>. Terrestrial ecosystems contributed insignificantly to XCO<sub>2</sub> in other months (<0.39 ppm). The annual mean biogenic contributions to XCO<sub>2</sub> in Northeast China in 2016 was estimated to be –0.60 ppm, which offsets 71% of the annual mean positive anthropogenic contribution (0.84 ppm).

### 3.4. Diurnal Variations of NEE and Surface CO<sub>2</sub> Concentrations

Source and sinks of CO<sub>2</sub> at regional to continental scales remain poorly understood. Even though multiple GPP products on daily scales (usually 8-day) are available, their performances vary substantially when



**Figure 11.** Mean diurnal variation of the NEE spread during the growing season (May through September) in 2016 from multiparameter ensemble simulation (ES1, shaded area) and mean and standard deviation (error bars) values of NEE from single-parameter simulations ( $\alpha$ , triangle;  $\beta$ , line;  $\lambda$ , circle; and  $PAR_0$ , diamond) at Wuying mixed forest station at 03:00, 08:00, 12:00, 17:00, and 21:00 BT. Thick black line represents observed NEE at Wuying site, and gray line represents simulated NEE with WRF-VPRM.



**Figure 12.** Scattering plots of differences between the growing-season-averaged NEE values for each member in ensemble simulations and that simulated with WRF-VPRM at Wuying against relative variation ratio of VPRM parameters (including  $\alpha$ ,  $\beta$ ,  $\lambda$ , and  $PAR_0$ ). (a–d) multiparameter ensemble simulations (ES1); (e–h) single-parameter simulation (ES2–ES5).

validated against EC observations (Zhang et al., 2017b). This is at least partly due to our limited understanding on the photosynthesis and respiration processes, including their diurnal variations. Better estimation of total NEE has to be achieved through better understanding of its diurnal variation and better parameterization of diurnal variations of the photosynthesis and respiration processes. Diurnal variation of  $CO_2$  fluxes and concentration was examined below.

The observed diurnal variation pattern of NEE and surface  $CO_2$  concentrations at Fujin and Wuying (Figure 10) was consistent with previous observations (Bazzaz & Williams, 1991; Guan et al., 2006; Park et al., 2018; Song et al., 2006; Zhang et al., 2017a). The negative NEE occurred between 06:00 and 17:00 BT, with the lowest value at the middle of the day, while the surface  $CO_2$  concentration began to increase after sunset, reached a peak in the early morning, and then decrease till 18:00 BT at both stations.

The observed mean diurnal variation of NEE in the growing season exhibited a wider range in mixed forest (from  $-12.8$  to  $3.6 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  at Wuying; see Figure 10b) than the rice paddy field (from  $-9.2$  to  $2.2 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  at Fujin; see Figure 10a). This suggests mixed forests acted as a larger  $CO_2$  sink/source than rice paddies in 2016 due to a longer growth period and stronger ER, although the canopy photosynthesis and hence the peak  $CO_2$  sink were stronger in rice paddies in June and July (Figures 3a and 4a). These differences corroborate previous understanding that terrestrial ecosystems with the greatest net carbon uptake usually have the longest growing season, rather than the greatest canopy photosynthesis (Baldochi, 2008). The nighttime EC-measured NEE at Wuying ( $>3 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) was larger than that at Fujin ( $<2 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) likely because of stronger soil respiration in forest than that in rice paddy (Brændholt et al., 2018; Ren et al., 2007; Tang et al., 2008), as well as stronger leaf and stem respiration in forests than in rice paddies due to the difference in biomass. The mean EVI during the growing season at Wuying was approximately 30% higher than that at Fujin in 2016 (Figures 3c and 4c). The growing-season mean diurnal variation of surface  $CO_2$  concentration at Wuying also exhibited a wider range than that at Fujin (Figures 10b and 10d), which is partially due to larger  $CO_2$  fluxes at mixed forest.

Different from many previous LUE model investigations that examined daily mean surface  $CO_2$  fluxes (Running et al., 2004; Xiao et al., 2008; Zhang et al., 2017b), our online WRF-VPRM simulation calculates  $CO_2$  fluxes and three-dimensional  $CO_2$  fields every time step. Thus, we can examine  $CO_2$  fluxes and concentrations on a subdaily time scale using WRF-VPRM outputs and examine model errors on short time scales that have not been thoroughly discussed before (Diao et al., 2015; Zhang et al., 2017a). WRF-VPRM well reproduced the daytime NEE and surface  $CO_2$  concentration at Fujin but slightly overestimated their nighttime values (Figures 10a and 10c). At Wuying, the model overestimated the daytime NEE by approximately 9% ( $\sim 2.25 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) and underestimated the nighttime NEE by 38% ( $\sim 0.66 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ) on average (Figure 10b). As a result, the diurnal variation range of surface  $CO_2$  concentrations at Wuying was also underestimated (Figure 9d). Zhang et al. (Zhang et al., 2017a) also reported an underestimation on diurnal variation of NEE simulated with VPRM in the growing season in a mixed

**Table 4**  
*Values of Maximum Light Use Efficiency  $\lambda$  Optimized Over Different Mixed Forests in Previous Studies*

Reference	Site location	Observational year	Values of $\lambda$
Hilton et al. (2013)	North America	2007	0.20
Zhang et al. (2017)	Changbaishan, Northeast China	2015	0.315
Dayalu et al. (2018)	Changbaishan, Northeast China	2015	0.123
Yuan et al. (2013)	Global 9 sites	—	$2.03 \pm 0.24$
Mahadevan et al. (2008)	Massachusetts, United State	2000–2003	0.127
Mahadevan et al. (2008)	Maine, United State	2000–2003	0.123

forest region of the Changbai Mountains using default VPRM parameters from Mahadevan et al. (2008). In order to understand the model performance at Wuying, we conducted off-line VPRM sensitivity simulations to understand the uncertainty of NEE simulation in relation to the selection of VPRM parameters in the next section.

### 3.5. Parametric Uncertainty Analysis of NEE Simulations Using Off-Line VPRM

We conducted five experiments with off-line VPRM ensemble simulations (ES1–ES5, designed in section 2.4) at Wuying during the growing season of 2016 to investigate the uncertainty of NEE simulations in relation to the choices of VPRM parameters. The sensitivity of NEE in the daytime was larger than at nighttime. The NEE ranges in multiparameter run (ES1) covered the observed NEE at all hours during the growing season, showing that the WRF-VPRM is able to predict the observed NEE through adjusting the VPRM parameters. The results of ES2–ES5 suggested that the nighttime NEE depended more on  $\alpha$  than on  $\beta$ ; while the daytime NEE depended more on  $\lambda$  and  $PAR_0$  than on two respiration parameters (Figure 11).

The sensitivity of NEE to each VPRM parameter is shown in Figure 12. We calculated the differences between the growing-season averaged NEE for each member from ES1–ES5 and from the WRF-VPRM simulation. Figure 12 shows the relationships of these NEE differences against the relative variation ratio of each VPRM parameter. In ES1, the NEE differences exhibited strong negative correlations with variation of  $\lambda$  and  $PAR_0$ , a weak positive correlation for  $\alpha$ , and no obvious correlation for  $\beta$ . This means during the growing season, photosynthesis process dominantly controlled the NEE. In ES2–ES5, the NEE difference was most sensitive to  $\lambda$ , followed by  $PAR_0$ ,  $\alpha$ , and  $\beta$ . This means a small change of  $\lambda$  can lead to a considerable variation of simulated NEE.

The  $\lambda$  is commonly known as an important parameter to calculate GEE and then NEE in the VPRM (Liu et al., 2015); however, the literature shows a large range of possible values (see Table 4). The large uncertainties and diversities of estimates of  $\lambda$  are due to the difference in climatic environment at different observational sites, data processing procedure, and driving data used. Such parametric uncertainties in WRF-VPRM can be probably reduced by more detailed classification of land use based on MODIS data and calibrating these VPRM parameters over these more detailed land use categories, given that more detailed land classification based on MODIS data is reliable and tower data are available for the detailed land use classification. However, currently, both the prerequisites for such improvement of WRF-VPRM (i.e., more detailed land use classification based on MODIS and tower data over each detailed land use classification) are not very realistic, particularly over Northeast China where tower data are very sparse. Under such circumstances, ensemble simulations help to predict a better range of NEE as long as a reasonable range for each parameter can be provided. The sensitivity analysis based on ensemble simulations also provides guidance for future studies, suggesting that the best parameter to optimize would be  $\lambda$ . Global optimization of VPRM parameters is beyond the scope of the current project but should be revisited in the future.

## 4. Conclusions

Northeast China is dominated by mixed forest and cropland with prominent terrestrial  $CO_2$  fluxes. Long-term  $CO_2$  fluxes and their impacts on  $CO_2$  concentrations are poorly understood for this region. In this study, the terrestrial  $CO_2$  fluxes and concentrations in Northeast China during 2016 are analyzed using (1) field measurements at a rice paddy site in Fujin and a mixed forest site in Wuying, (2) satellite observations, and (3) the online WRF-VPRM simulation. To the best of our knowledge, the present work is the first one to

study the CO<sub>2</sub> sources/sinks and budget in Northeast China using an online WRF-VPRM simulation together with field and satellite observations.

The seasonal variations of NEE and surface CO<sub>2</sub> concentrations were first examined. Negative NEE (i.e., uptake of CO<sub>2</sub>), corresponding to high EVI, mostly occurred from mid-July to September at the Fujin rice station, and from May to September at the Wuying forest station. The lowest daily mean NEE occurred in August with  $-10 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  at Fujin, and in July with  $-6.5 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$  at Wuying, respectively. During the nongrowing season, when the EVI was low, the NEE remained negligible at both stations. The seasonal variations of surface CO<sub>2</sub> concentrations were greatly influenced by terrestrial CO<sub>2</sub> fluxes, with the lowest value in summer. WRF-VPRM reproduced the seasonal variations of NEE and surface CO<sub>2</sub> concentrations, with a better performance at Fujin than Wuying. The NEE at Wuying was overestimated on average during the growing season (May through September) due to the overestimation of GEE. VPRM does not consider the impact of biomass on respiration and sets ER as zero when  $T_a < -\beta/\alpha$ , which should be improved in the future. Notwithstanding, the WRF-VPRM also successfully captured a high surface CO<sub>2</sub> episode in the nongrowing season on October 15. This episode occurred due to the transport of CO<sub>2</sub> by strong southwesterly winds and subsidence as well as enhanced local biotic respiration due to an abrupt increase in  $T_a$ .

In addition to near-surface variables, we also examined the total column abundance of CO<sub>2</sub> (XCO<sub>2</sub>). The simulated monthly XCO<sub>2</sub> by WRF-VPRM was comparable to the OCO-2 observations, with the lowest value (395 ppm) in summer and the highest value (406 ppm) in spring. The annual anthropogenic and biogenic contributions to XCO<sub>2</sub> over Northeast China in 2016 were estimated to be approximately 0.84 and  $-0.60$  ppm, respectively, based on WRF-VPRM outputs.

The mean diurnal variations of NEE and surface CO<sub>2</sub> concentrations were examined at Fujin and Wuying during the growing season. The mean diurnal variation ranges of NEE and surface CO<sub>2</sub> concentrations were larger at Wuying than at Fujin because of stronger ER and longer growth period of mixed forest compared to those of rice paddy. WRF-VPRM reproduced the daytime NEE and CO<sub>2</sub> concentrations at Fujin well but slightly underestimated their nighttime value by  $1.05 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ , on average. The model significantly underestimated the diurnal variation ranges of NEE and surface CO<sub>2</sub> concentrations at Wuying forest station.

To investigate the uncertainties of VPRM parameters in relation to NEE error over Wuying, one multiparameter (ES1) and four single-parameter (ES2–ES5) ensemble simulations were conducted for the growing season with off-line VPRM. The variation range of simulated NEE in ES1 enveloped the observed NEE at all hours during the growing season. The nighttime NEE was more sensitive to  $\alpha$  than  $\beta$ , while the daytime NEE was most sensitive to  $\lambda$ . As a major source for the reducible uncertainties in WRF-VPRM, the uncertainties in the four VPRM empirical parameters can be reduced through optimization using more observational data in the studied region. Given the current uncertainties of these parameters, ensemble simulation perturbing the parameters in their plausible range is another method to capture the range of NEE and subsequent CO<sub>2</sub> transport and dispersion.

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