Implementation of improved parameterization of terrestrial flux in WRF-VPRM improves the simulation of nighttime CO2 peaks and a daytime CO2 band ahead of a cold front

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Abstract

Enhanced CO2 mole fraction bands were often observed immediately ahead of cold front during the Atmospheric Carbon and Transport (ACT)-America mission and their formation mechanism is undetermined. Improved understanding and correct simulation of these CO2 bands are needed for unbiased inverse CO2 flux estimation. Such CO2 bands are hypothesized to be related to nighttime CO2 respiration and investigated in this study using WRF-VPRM, a weather-biosphere-online-coupled model, in which the biogenic fluxes are handled by the Vegetation Photosynthesis and Respiration Model (VPRM). While the default VPRM satisfactorily parameterizes gross ecosystem exchange, its treatment of terrestrial respiration as a linear function of temperature was inadequate as respiration is a nonlinear function of temperature and also depends on the amount of biomass and soil wetness. An improved ecosystem respiration parameterization including enhanced vegetation index, a water stress factor, and a quadratic temperature dependence is incorporated into WRF-VPRM and evaluated in a year-long simulation before applied to the investigation of the frontal CO2 band on 4 August 2016. The evaluation shows that the modified WRF-VPRM increases ecosystem respiration during the growing season, and improves model skill in reproducing nighttime near-surface CO2 peaks. A nested-domain WRF-VPRM simulation is able to capture the main characteristics of the 4 August CO2 band and informs its formation mechanism. Nighttime terrestrial respiration leads to accumulation of near-surface CO2 in the region. As the cold front carrying low-CO2 air moves southeastward, and strong photosynthesis depletes CO2 further southeast of the front, a CO2 band develops immediately ahead of the front.

Implementation of improved parameterization of terrestrial flux in WRF-VPRM improves the simulation of nighttime CO_2 peaks and a daytime CO_2 band ahead of a cold front

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Key Points

1. A new terrestrial ecosystem respiration parameterization accounting for vegetation index, water stress, and a nonlinear temperature dependence is implemented in WRF-VPRM to improve the simulation of both respiration and GPP.
2. The daytime bands of elevated CO_2 mole fractions ahead of cold fronts form in part due to the accumulation of nighttime respiration; hence the new VPRM improves performance.
3. Cloud-shading induced perturbation of photosynthesis cannot explain the CO_2 band immediately ahead of the surface cold front on 4 August 2016 because of its small magnitude and lagging behind the front.
4. Biological CO_2 clearly dominates the lower tropospheric CO_2 mole fraction patterns on the synoptic scale, with cross-frontal variations of more than 30 ppm for photosynthesis and respiration.

Abstract

Enhanced CO_2 mole fraction bands were often observed immediately ahead of cold front during the Atmospheric Carbon and Transport (ACT)-America mission and their formation mechanism is undetermined. Improved understanding and correct simulation of these CO_2 bands are needed for unbiased inverse CO_2 flux estimation. Such CO_2 bands are hypothesized to be related to nighttime CO_2 respiration and investigated in this study using WRF-VPRM, a weather-biosphere-online-coupled model, in which the biogenic fluxes are handled by the Vegetation Photosynthesis and Respiration Model (VPRM). While the default VPRM satisfactorily parameterizes gross ecosystem exchange, its treatment of terrestrial respiration as a linear function of temperature was inadequate as respiration is a nonlinear function of temperature and also depends on the amount of biomass and soil wetness. An improved ecosystem respiration parameterization including enhanced vegetation index, a water stress factor, and a quadratic temperature dependence is incorporated into WRF-VPRM and evaluated in a year-long simulation before applied to the investigation of the frontal CO_2 band on 4 August 2016. The evaluation shows that the modified WRF-VPRM increases ecosystem respiration during the growing season, and improves model skill in reproducing nighttime near-surface CO_2 peaks. A nested-domain WRF-VPRM simulation is able to capture the main characteristics of the 4 August CO_2 band and informs its formation mechanism. Nighttime terrestrial respiration leads to accumulation of near-surface CO_2 in the region. As the cold front carrying low-CO_2 air moves southeastward, and strong photosynthesis depletes CO_2 further southeast of the front, a CO_2 band develops immediately ahead of the front.

1. Introduction

An enhanced CO_2 mole fraction band was often observed immediately ahead of cold fronts during the Atmospheric Carbon and Transport (ACT)-America mission (Pal et al., 2020). Correct simulation of the gradients of CO_2 across cold fronts and understanding of the formation mechanisms are needed for accurate estimation of regional CO_2 budget (Chan et al., 2004; Hurwitz et al., 2004; Lee et al., 2012; Pal et al., 2020; Parazoo et al., 2008). Improved understanding of atmospheric constituents including CO_2 ahead of fronts may also help explain air pollution events sometimes found ahead of fronts (Hu et al., 2019a) since CO_2 and pollutants are sometimes co-emitted (Brioude et al., 2013; Brioude et al., 2012; Konovalov et al., 2014; Lindenmaier et al., 2014; Reuter et al., 2019; Turnbull et al., 2011; Wunch et al., 2009; Yang et al., 2019a). These CO_2 bands were previously briefly examined using WRF-VPRM, a weather-biosphere-online-coupled model, in which the terrestrial fluxes are handled by the Vegetation Photosynthesis and Respiration Model (VPRM) while the Weather Research and Forecast (WRF) model (Skamarock et al., 2008; Skamarock & Klemp, 2008) is used to simulate atmospheric flows and CO_2 transport and diffusion. These previous WRF-VPRM simulations were able to capture the existence of the CO_2 bands during the ACT-America mission (Hu et al., 2020a). However substantial bias in terms of CO_2 magnitude existed, which appeared related to underestimation of diurnal variation of CO_2, particularly nighttime CO_2 peaks (Li et al., 2020; Wang et al., 2020). Other studies also implied that VPRM and WRF-VPRM tended to underestimate nighttime CO_2 fluxes (Dayalu et al., 2018; Lopez-Coto et al., 2017) and concentration (Park et al., 2020). Nighttime CO_2 biases were not extensively examined previously. Many previous regional CO_2 studies focused on daytime boundary layer CO_2, while nighttime CO_2 was less studied (Parazoo et al., 2008), likely because of two factors: 1, nighttime CO_2 simulations are less trusted because of uncertainties in the parameterization of the nighttime boundary layer and terrestrial respiration fluxes; 2, many remote-sensing and in-situ (such as aircraft) CO_2 observations are only available during daytime (Crevoisier et al., 2010; Pal et al., 2020; Sweeney et al., 2015).

Terrestrial ecosystem respiration in simple empirical modeling systems such as VPRM is often parameterized as a function of temperature, thus not accounting for factors such as soil moisture and substrate available for heterotrophic respiration (Ai et al., 2020; Buchmann, 2000; Fang & Moncrieff, 2001; Lloyd & Taylor, 1994; Raich et al., 2002; Schubert et al., 2010). VPRM simulates the Net Ecosystem Exchange (NEE) of CO_2 through separate parameterizations for ecosystem respiration (ER) and Gross Ecosystem Exchange (GEE) (Mahadevan et al., 2008)

$$\mathrm{NEE} = \mathrm{ER} + \mathrm{GEE} \tag{1}$$
$$\mathrm{ER} = \alpha \times T + \beta \tag{2}$$
$$\mathrm{GEE} = \lambda \times T_{scale} \times W_{scale} \times P_{scale} \times FAPAR_{PAV} \times PAR \times \frac{1}{1+\frac{PAR}{PAR_0}} \quad , \tag{3}$$

where α and β are parameters used to model ecosystem respiration as a function of temperature T, λ is the maximum light use efficiency, T_{scale}, W_{scale}, and P_{scale} account for effects of temperature, water stress, and leaf age on photosynthesis, respectively, $FAPAR_{PAV}$ is the Fraction of Photosynthetically Active Radiation (PAR, μmol m^{-2} s^{-1}) absorbed by the photosynthetically-active portion of the vegetation, which roughly equals the Enhanced Vegetation Index (EVI), and PAR_0 is the half-saturation value. This version of VPRM (Mahadevan et al., 2008) and the corresponding parameters previously calibrated off-line using eddy covariance tower data over North America (Hilton et al., 2016) were implemented into WRF-VPRM to examine spatiotemporal variation of CO_2 over the contiguous U.S. (Hu et al., 2020b) and northeastern China (Li et al., 2020). While Eq. (3) is a light-use efficiency algorithm commonly used to simulate GEE (Dong et al., 2015; Wagle et al., 2014; Zhang et al., 2016a; Zhang et al., 2016b; Zhang et al., 2018; Zhang et al., 2017), respiration (Eq. 2), is considerably simpler than parameterizations of ecosystem respiration in more complex, process-based models. Ecosystem respiration depends not only on temperature but also on other factors such as soil moisture (Davidson et al., 1998; Murayama et al., 2003; Rey et al., 2002) and the mass of leaf and stem of biomes (proxy of plant productivity) that can be roughly represented by EVI (Guan et al., 2006). The leaf and stem respiration (which is the dominant contributor to autotrophic respiration) was observed to account for about 27%-52% of the total ecosystem respiration on annual average, with a higher percentage during summer (Guan et al., 2006; Tang et al., 2008). Biogeochemical models like Carnegie Ames Stanford Approach (CASA) (Zhou et al., 2020) and Simple Biosphere Model (SiB4) (Haynes et al., 2019) track carbon pools, and simulate respiration as a function of the carbon pool size, along with pool-specific litter decay rates and environmental controlling factors. Other studies (Loranty et al., 2011) attempted to include plant productivity in ecosystem respiration parameterization by making respiration a function of leaf area index. A better respiration parameterization is warranted for improving WRF-VPRM.

Recently an improved terrestrial respiration parameterization in VPRM has been developed by incorporating EVI, water stress scaling factor (W_{scale}) and its interactions with temperature to capture soil moisture effects, and a quadratic dependence on surface air temperature (T in °C) (Gourdji et al., 2020):

$$ER = \beta + \alpha_1 \cdot T + \alpha_2 \cdot T^2 + \gamma \cdot EVI + k_1 \cdot W_{scale} + k_2 \cdot W_{scale} \cdot T + k_3 \cdot W_{scale} \cdot T^2 \quad (4)$$

The parameters in this improved VPRM (Eq. 3 and 4) were calibrated with comprehensive flux tower data. Preliminary evaluation showed that this improved parameterization leads to better prediction of diurnal and monthly variation of CO_2 fluxes and concentration (Gourdji et al., 2020). This improved respiration parameterization is implemented into WRF-VPRM in this study and its performance over the contiguous United States (CONUS) is evaluated in 2016, particularly in terms of reproducing nighttime boundary layer CO_2 at six NOAA towers (see their locations in Fig. 1), where hourly in-situ boundary layer CO_2 data are available in both daytime and nighttime. High-resolution simulations with this improved WRF-VPRM is further used to examine the CO_2 band ahead of the cold front on 4 August 2016 observed during the ACT-America aircraft field campaign, a case well documented previously using observations (Pal et al., 2020) and simulations.

2. Modeling approach and evaluation data

2.1 Brief description of VPRM improvement

The respiration parameterization of Eq. (4) is implemented into WRF-VPRM. While in the GEE calculation (Eq. 3), W_{scale} considers water stress effect using a function of Land Surface Water Index (LSWI):

$$W_{scale}(GEE) = \frac{1+LSWI}{1+LSWI_{max}} \tag{5}$$

following earlier VPRM development studies (Mahadevan et al., 2008; Xiao et al., 2004), W_{scale} used for ER calculation adopts

$$W_{scale}(ER) = \frac{LSWI-LSWI_{min}}{LSWI_{max}-LSWI_{min}} \tag{6}$$

proposed by Matross et al. (2006) for relatively-more water-limited region, because Eq. (6) leads to a larger variation of W_{scale} between different seasons with different water stresses. Eq. 6 was previously used for GEE calculation in grass and shrubs, but we change it to Eq. 5 to better match early growing season uptake in these ecosystems (Gourdji et al., 2020).

To maintain minimal terrestrial respiration in presence of low temperature in winter months and account for the fact that soil temperature is higher than air temperature during winter, the temperature (in °C) used in Eq. (4) is adjusted to

$$T = (T_a - T_{crit}) \cdot T_{scale2} + T_{crit} \tag{7}$$

when the air temperature T_a is lower than T_{crit}. The VPRM parameters (GEE and respiration parameters in Eq. 3, 4, and T_{scale2} and T_{crit} in Eq. 7) for each vegetation type are summarized in Table 1, and were calibrated by Gourdji et al., (2020) using AmeriFlux data (*https://ameriflux.lbl.gov/sites*). Respiration parameters were first calibrated using nighttime data, and then daytime respiration were computed, and daytime GEE were separated out, which was subsequently used to optimize GEE parameters. This is a different optimization procedure than originally formulated by Mahadevan et al (2008), where 24 hours of hourly NEE are used to simultaneously optimize GEE and respiration parameters. The new optimization procedure results in a larger magnitude of both respiration and GEE, and hence the diurnal cycle of NEE, by separately fitting respiration and GEE parameters to night and day-time observations respectively. A more detailed description of the improved VPRM and parameter calibration can be found in Gourdji et al. (2020), although parameters for western shrubs and grasslands were optimized separately for the simulations presented in this study, given that Gourdji et al. (2020) focuses on estimating fluxes in eastern North America.

2.2 Configurations of WRF-VPRM simulations and episode description

Two kinds of WRF-VPRM simulations, referred to as year-long and episodic, are conducted. A single-domain, one year WRF-VPRM downscaling simulation is conducted over the CONUS domain at a 12-km grid spacing in 2016 to examine the updated VPRM performance over a full year. Following the year-long run, nested-domain episodic WRF-VPRM simulations are conducted for 4 August 2016 to examine the formation mechanism of the CO_2 band ahead of the cold front at a higher horizontal resolution, with an inner nested domain covering the northern Great Plains at a 4 km grid spacing (see domain configuration in Fig. 1).

The year-long WRF-VPRM simulation follows the configuration of our previous downscaling study (Hu et al., 2020b), with the NCEP/DOE R2 data (Kanamitsu et al., 2002) providing meteorological initial and boundary conditions and the CT2017 global simulation 3°×2° outputs (Peters et al., 2007) providing CO_2 initial and boundary conditions. Anthropogenic CO_2 emissions are taken from the 0.1°×0.1° Open-Data Inventory for Anthropogenic Carbon dioxide (ODIAC) (Oda et al., 2018) version 2018 and ocean CO_2 fluxes are taken from climatological monthly values derived by Takahashi et al. (2009). Using ODIAC led to a better CO_2 simulation than using Emission Database for Global Atmospheric Research (EDGAR) in Hu et al. (2020b). Selected major physics parameterization schemes within WRF include the Dudhia shortwave radiation scheme (Dudhia, 1989), the rapid radiative transfer model (RRTM) (Mlawer et al., 1997) for longwave radiation, the Noah land surface model (Chen & Dudhia, 2001), the Grell-3 cumulus scheme (Grell & Devenyi, 2002), the Morrison microphysics scheme (Morrison et al., 2009), and the Yonsei University (YSU) planetary boundary layer (PBL) scheme (Hong et al., 2006). Selection of PBL schemes is critical for accurate simulation of lower tropospheric CO_2 vertical distribution (Ballav et al., 2016; Diaz-Isaac et al., 2018) and CO_2 accumulation ahead of cold fronts. The YSU scheme has been shown to perform well for both daytime and nighttime at the 12 and 4 km grid spacings used in this study (e.g., Hu et al., 2012; Hu et al., 2013; Hu et al., 2010b; Hu et al., 2019b; Yang et al., 2019b). The YSU scheme is a nonlocal scheme with explicit treatment of entrainment fluxes, which was shown to be critical to reproducing convective boundary layer structures (Hu et al., 2010b; Hu et al., 2019b) and achieve a better performance than some local schemes such as the Mellor–Yamada–Janjic (MYJ) scheme (Wang et al., 2016). For stable boundary layer, an update in stability function in 2013 led to a better YSU performance in terms of reproducing nighttime profiles of both meteorological and chemical variables, particularly over the Great Plains (Hu et al., 2013). The model domain has 47 vertical layers extending from the surface to 10 hPa with 21 layers in the lower 2 km above the ground to resolve boundary layer processes. The WRF-VPRM downscaling simulation ran continuously from January 1 to December 31, 2016, adopting the spectral nudging technique (Gomez & Miguez-Macho, 2017; Otte et al., 2012; Vincent & Hahmann, 2015) to ensure that the large scale flows do not deviate from the driving NCEP/DOE R2 data, following our previous downscaling studies (Hu et al., 2020b; Hu et al., 2017; Hu et al., 2018). Such long-term regional simulations refine global model simulation (CT2017 in this case) and improve the general accuracy of simulation by better resolving local forcing and atmospheric processes, and are commonly referred to as dynamic downscaling.

The nested-domain simulations for 4 August 2016 examine the formation mechanism of the CO_2 band ahead of the cold front on the nested 4 km grid. During the selected episode, a surface cold front that formed on 3 August moved southeastward quickly to central Nebraska until 12 CST (18 UTC) 4 August when it slowed down (Pal et al., 2020). Along the front, scattered light clouds were present and at some isolated points/time there were large thunderstorms, e.g., at Lincoln after landing of ACT research flight. OCO-2 XCO_2 data indicate a transition of low XCO_2 to high XCO_2 across the front (Fig. 1c). But due to the interference of clouds, OCO-2 could not detect the detailed gradient across the front (Bell et al., 2020; O'Dell et al., 2018). Lower troposphere measurements from the ACT-America flight campaign reveal an enhanced CO_2 mole fraction band (~50 km wide) immediately ahead of the cold front with the cross-frontal CO_2 contrast as high as 30 ppm (Pal et al., 2020). Note ppm is equivalent to µmol/mol. These CO_2 bands formed likely due to a few factors including horizontal and vertical transport, and reduced photosynthetic uptake caused by clouds (Chan et al., 2004; Hu et al., 2020a; Lee et al., 2012). The finer horizontal and vertical resolutions used in this study can better resolve small-scale processes and shallow surface layers than earlier studies using coarse resolutions (e.g., Chan et al., 2004), which is critical for reproducing the formation of the narrow CO_2 bands. To diagnose the CO_2 band, in addition to the fully coupled control run, two sensitivity simulations (summarized in Table 2) are conducted, in which clear-sky radiation is used to drive VPRM and the Noah land surface model, respectively. These sensitivity simulations are designed to isolate the impact of cloud shading on terrestrial CO_2 fluxes and surface energy balance, respectively, and the subsequent impact on frontal CO_2 structures.

2.3 Description of Observations

2.3.1 NOAA Tall Towers

Hourly data from six NOAA tall towers over central and eastern half of US, i.e., WLEF Tower (LEF), Argyle, Maine Tower (AMT), West Branch, Iowa (WBI), South Carolina Tower (SCT), Boulder Atmospheric Observatory (BAO), and WKT Tower (WKT), are used to evaluate simulated CO_2 profiles in the continental boundary layer during both daytime and nighttime. The measurements at BAO were discontinued on 26 July 2016. More detailed description of those towers can be found at https://www.esrl.noaa.gov/gmd/ccgg/insitu/.

2.3.2 Atmospheric Carbon and Transport (ACT)-America data

The ACT-America mission was conducted to improve the understanding of sources and sinks of CO_2 at regional scale (~10^6 km^2) and transport of greenhouse gases by weather systems in midlatitudes. During the mission, two aircraft (NASA Wallops C130 - Hercules and NASA Langley B200 – King Air) were deployed over the eastern half of the continental U.S. during 2016-2019, to measure meteorological variables and gas species including CO_2 and CH_4 across a variety of weather conditions in both the boundary layer and the free troposphere (Davis et al., 2018;

Digangi et al., 2018). Airborne CO_2 were measured using a PICARRO 2401-m analyzer calibrated with gas standards traceable to the WMO scale. The ACT-America flight data on 4 August 2016 (see flight track of B200 in Fig. 1) are used in this study to evaluate the CO_2 simulation with the updated WRF-VPRM and to examine the CO_2 band ahead of the cold front.

3. Results

3.1 Evaluation of year-long CO_2 downscaling simulation with tower data

The year-long WRF-VPRM downscaling simulation is conducted mainly to examine the performance of the updated VPRM, particularly in terms of reproducing nighttime boundary layer CO_2 peaks, because nighttime CO_2 was found to contribute substantially to the daytime CO_2 bands ahead of cold fronts (Hu et al., 2020a). Note that the effect of simulated CO_2 variations on radiation and subsequent weather is not considered in current WRF-VPRM (such effect should be much smaller than meteorological conditions such as clouds, atmospheric temperature and water vapor distributions (Houghton & Moir, 1977)). Instead, a climatological CO_2 mole fraction (379 ppm) is used in the radiation scheme. Thus, updates in VPRM do not affect the simulated meteorological fields, which are essentially the same as those reported in Hu et al. (2020b). Comprehensive evaluation conducted in Hu et al. (2020b) concluded that the downscaled meteorological fields are sufficiently accurate to drive online coupled VPRM and subsequent CO_2 simulation.

The updated VPRM predicts enhanced respiration during growing season, partially due to added dependence on EVI. While a more detailed evaluation of VPRM fluxes can be found in a companion paper (Gourdji et al., 2020), CO_2 fluxes at an AmeriFlux site (US-Ne3, see its location in Fig. 1) near the B200 flight track are evaluated in Fig. 2. During non-growing season, both model and observations show minimal NEE except observations show occasional spikes. During growing season at this crop site (July, August, September), both negative and positive CO_2 fluxes are enhanced, indicating daytime NEE and nighttime ER, respectively. The previous version of VPRM with Eq. (2) underestimates growing season NEE and ER (Fig. 2a,c). With the modified ER parameterization (Eq. 4) and newly calibrated parameters, the updated VPRM (referred to as VPRM_G in figure legends) predicts enhanced productivity with enhanced NEE during both daytime and nighttime during growing season, showing a better agreement with observations (Fig. 2b,d). The growing season mean bias of nighttime CO_2 fluxes is reduced from -4.2 to -0.2 μmol CO_2 m^{-2} s^{-1} at this site, which is a critical improvement to reproducing the daytime CO_2 bands ahead of cold front as will be discussed in section 3.2. Different from simulated fluxes, which represent the average flux over a 12×12 km^2 grid cell, observed fluxes represent the flux at the site and observed nighttime fluxes often show positive spikes (Fig. 2a,b) presumably due to instantaneous intermittent turbulence particularly during growing season (Aubinet, 2008). The median diurnal variation of CO_2 fluxes during growing season is evaluated in Fig. 2c,d, which further confirms that the new VPRM better captures the diurnal variation of fluxes relative to the old VPRM formulation. Examination of CO_2 fluxes at a grass site in Kansas close to the 4 August B200 flight track also indicates a better performance of the new VPRM (figure not shown).

Fluxes along with transport dictate the atmospheric CO_2 spatiotemporal variation. Simulated hourly CO_2 values at six NOAA tower sites are evaluated. Among the six sites, three northern sites, WBI (crop site) and LEF and AMT (mixed forest sites), show more pronounced seasonal variation of CO_2 (Fig. 3), indicating more pronounced seasonal cycle of productivity. The strong variation of hourly values in the growing season (Fig. 4) is due to enhanced diurnal variation of NEE relative to non-growing season. Detailed hourly variation of CO_2 in first half of July is shown in Fig. 5, illustrating intense diurnal variation with nighttime CO_2 peaks (grey shading) and afternoon CO_2 minima (no shading). Afternoon minimum CO_2 shows a prominent seasonal cycle with minimum in July-August at WBI crop site and in June-September at LEF, AMT mixed forest sites (Fig. 3), consistent with previous studies (Bakwin et al., 1998; Parazoo et al., 2008), indicating active terrestrial uptake in growing season during daytime. Note that mixed forest typically has a longer growing season than crop (Li et al., 2020). Such seasonal variation of afternoon minimum CO_2 also shows up in the aircraft boundary layer CO_2 data from NOAA Global Greenhouse Gas Reference Network (https://www.esrl.noaa.gov/gmd/ccgg/aircraft/) and the XCO_2 data recorded at Total Carbon Column Observing Network [TCCON] (Hu et al., 2020b), both of which only have daytime observations. Relatively-less-reported is the seasonal variation of nighttime CO_2 peaks/spikes (e.g., Bakwin et al., 1998; Davis et al., 2003), which increase significantly during growing seasons (Fig. 3). The increasing magnitude of nighttime CO_2 peaks/spikes during growing season is even larger than the decreasing magnitude of afternoon CO_2 minimum (Fig. 3).

For SCT and two grass sites, BAO, and WKT, the contrast between the non-growing season and growing season identified from time series of hourly CO_2 is not as clear as the crop and mixed forest sites, which is due to a smaller seasonal variation of local fluxes and location in the continent (Sweeney et al., 2015).

The updated VPRM showed improved performance compared to the previous version, particularly in terms of reproducing nighttime CO_2 peaks (Fig. 5). Overall, the underestimation of surface CO_2 is reduced, with 24-hour mean bias reducing from -5.3 ppm to -1.0 ppm at the six NOAA sites in 2016 (Table 3). During nighttime (22-06 CST) the mean bias is reduced from -9.4 ppm to -4.0 ppm (Table 5) while during the day (10-18 CST) the mean bias is changed from -1.1 ppm to 1.6 ppm (Table 4). The nighttime mean bias remains most prominent at two mixed forest sites, AMT (-10.4 ppm) and LEF (-4.4 ppm) with the updated VPRM (Fig. 3, Table 5). At the WBI crop site, nighttime mean bias reduced from -11.46 ppm to -4.2 ppm. The remaining bias at night could be due to overestimated nighttime turbulent mixing (Hu et al., 2010b), as well as underestimated nighttime respiration due to drainage and loss of measured flux at towers (Aubinet, 2008). These evaluations illustrate that the updated terrestrial respiration parameterization (i.e., Eq. 4) and the newly calibrated parameters (Table 1) have a much-improved skill to reproduce the nighttime CO_2 peaks, as well as diurnal variation of near-surface CO_2, particularly during growing season. Note that among the 6 NOAA towers, WBI is closest to the B200 flight track on 4 August 2016 and the flight track is mostly over the crop land category (Fig. 1a,b). Thus, significant improvement of WRF-VPRM performance over the WBI crop site is likely to be particularly beneficial to diagnose formation mechanism of the CO_2 band observed by B200 on 4 August.

In addition to terrestrial fluxes, the surface CO_2 concentration is dictated by boundary layer vertical distribution. Boundary layer CO_2 profiles are examined in Figs. 6-8 to further diagnose the CO_2 biases. During daytime (10, 14, 18 CST), CO_2 in the boundary layer is nearly well mixed, except at 18 CST when CO_2 starts to accumulate near the surface at eastern sites, e.g., AMT and SCT because these sites enter evening earlier comparing to western sites. The biases of these well-mixed daytime profiles are minor, consistent with previous evaluation using daytime measurements of boundary layer CO_2 from NOAA small aircraft and XCO_2 from TCCON (Hu et al., 2020b).

Comparing to daytime, biases of nighttime boundary layer CO_2 are relatively-less-reported. Through the night and the following early morning (22, 2, 6 CST), CO_2 from terrestrial respiration keeps accumulating near the surface in presence of a stable boundary layer and near-surface vertical gradients of CO_2 increase. Comparing to daytime, WRF-VPRM has more challenge to reproduce the nighttime CO_2 peaks. The bias of near-surface CO_2 becomes prominent during nighttime. With increased nighttime respiration in the updated VPRM (Eq. 4), the nighttime bias is alleviated. However, the bias of early morning CO_2 at certain sites are still large. For example, at AMT, the bias reaches as large as >20 ppm at 2 CST and the bias quickly reduces to <10 ppm at 6 CST as the convective boundary layer starts to grow and photosynthesis becomes active at this eastern site, reducing surface-layer CO_2 peaks quickly (Fig. 6). At 6 CST, the bias of surface CO_2 at WBI and LEF reaches ~16 ppm and 10 ppm, and the biases at three other south sites, SCT, BAO, WKT are smaller. The median diurnal variations of CO_2 during growing season (Fig. 4) also illustrate the largest nighttime bias remains at AMT, WBI, and LEF. Future further improvement of simulating boundary layer CO_2 diurnal variation may focus on the biologically very productive sites such as WBI crop site and AMT, LEF mixed forest sites, and may benefit from co-located measurements of fluxes, mole fraction, and boundary layer meteorology (Davis et al., 2003; Yi et al., 2004; Yi et al., 2001).

3.2 Examination of the CO_2 band ahead of cold front on 4 August 2016

3.2.1 Analysis of ACT-America data and fully coupled WRF-VPRM control simulation

An important purpose of this study is to examine the cause of elevated CO_2 bands ahead of cold fronts, which appeared to be related to nighttime accumulation of near-surface CO_2 (Hu et al., 2020a). With improved capability to reproduce the nighttime CO_2 surface flux and mole fraction peaks with the updated VPRM, we seek to better diagnose the formation mechanism of the CO_2 bands. The CO_2 band ahead of the cold front on 4 August 2016 is examined with nested-domain WRF-VPRM simulations (see domain configuration in Fig. 1). In early morning (0600 CST), the model captures the stable boundary layer structure, as verified by routine sounding data at KLBF, KOAX, and KTOP in the vicinity of the ACT-America flight track on this day (Fig. 9).

At 1000 CST when C130 took off, the convective boundary layer grew up to ~ 700 m AGL, as indicated by the potential temperature profile measured by C130 (Fig. 9b). Nighttime accumulated CO_2 in the stable boundary layer was mixed in this early shallow convective boundary layer with a vertically constant mole fraction of ~418 ppm, about 14 ppm higher than the CO_2 mole fraction in the free troposphere above (Fig. 9a). The control WRF-VPRM simulation captures these boundary layer structures even though certain biases exist, including overestimation of boundary layer potential temperature by 2-3 K and underestimation of boundary layer CO_2 with a mean bias of ~5 ppm. During the morning, the cold front kept pushing southeastward bringing the low-CO_2 air mass (indicated by the OCO-2 XCO_2 data in Fig. 1c and aircraft data in Fig. 10a,b) into the region. Meanwhile, enhanced GEE over cropland around Lincoln and area east of Lincoln (partially due to large EVI in the region, Fig. 1a) reduced the boundary layer CO_2, leading to formation of a high CO_2 mole fraction band between west of Lincoln and leading edge of the cold front, which was detected by B200 at ~1230 CST when it flew westward and crossed the front (Fig. 10). The WRF-VPRM simulation captures the CO_2 gradient across the front in both the boundary layer and free troposphere (Fig. 10b) and the horizontal variation of boundary layer CO_2 mole fraction along the B200 flight track, including the CO_2 band immediately ahead of the cold front and west of Lincoln, albeit the band position is a little off (Fig. 10a,b), which is partially due to the time difference between observation and simulation. The CO_2 band was observed at ~1230 CST while the simulation is taken at 1200 CST in Fig. 10 (WRF outputted hourly).

Simulated individual components of CO_2 in the higher-resolution inner domain are examined to further diagnose the CO_2 band attribution. Total CO_2 are decomposed into background, biogenic, anthropogenic, and oceanic CO_2, which are tracked by individual tracer in WRF-VPRM. While biogenic, anthropogenic, and oceanic CO_2 are CO_2 accumulated from the terrestrial biogenic fluxes, anthropogenic emissions and oceanic fluxes, background CO_2 is the CO_2 transported into the domain from the lateral boundary CO_2, which is derived from CT2017. Biogenic CO_2 can be further decomposed into respiration CO_2 and photosynthesis CO_2, which are CO_2 accumulated from transported ER and GEE, i.e., Eqs. (4) and (3). Among these components, oceanic CO_2 is negligible over the continent (Hu et al., 2020b) and therefore not shown here. The background CO_2 transported by the cold front has its origins from the northern boundary where CO_2 is low in summer (Hu et al., 2020b; Sweeney et al., 2015), thus southeastward penetration of background CO_2 carried by the cold front creates a step-function-like gradient (~6ppm difference) across the front, with a nearly constant CO_2 (~ 402 ppm) ahead of the cold front (Fig. 11b, 12b). The anthropogenic CO_2 includes a small contribution to CO_2 to the far east side along the B200 flight track, while it does not contribute to the CO_2 band immediately ahead of the cold front (Fig. 11d, 12d). The CO_2 enhancement band is mostly comprised of biogenic CO_2 (Fig. 11c), that is, accumulated from terrestrial biogenic fluxes, which contributes a ~15 ppm cross-front difference (Fig. 12c). The horizontal variation of biogenic CO_2 (Fig. 11c, 12c) matches the horizontal variation of total CO_2 (Fig. 11a, 12a) in terms of general trend.

Figure 12 also illustrates that updated VPRM significantly enhances the model capability to capture the CO_2 band ahead of the cold front. The previous version of VPRM, with a much weaker respiration given by Eq. (2), barely simulates any contribution to the cross-front CO_2 gradient from biogenic CO_2 at 12 CST, with only background CO_2 contributing a ~6ppm CO_2 gradient across the front. With a stronger respiration, updated WRF-VPRM simulates a dominating contribution from biogenic CO_2 (~15 ppm) to the cross-front CO_2 gradient, with certain biases still remaining including underestimating the peak concentration of the CO_2 band by ~8 ppm and overestimating the width of the CO_2 band.

To further delineate the effects of biogenic CO_2 fluxes, individual contribution history from respiration CO_2 and photosynthesis CO_2 during the morning of 4 August is examined in Fig. 13. In the early morning at 8 CST, respiration CO_2 ahead of the cold front is significant (~40 ppm) and does not show much variation along the B200 flight track (Fig. 13b). Photosynthesis CO_2 are enhanced (absolute value) over the cropland region with enhanced EVI (Fig. 1a) around Lincoln and area east of Lincoln (Fig. 13c). As a result of collective contribution of respiration and photosynthesis CO_2, biogenic CO_2 shows a band of enhanced mole fraction immediately ahead of the cold front (Fig. 13a). Through time, this CO_2 band is squeezed and pushed southeastward by the front, which was detected by B200 ~1230 CST (Fig. 13d). When the CO_2 band is pushed further into high GEE region east of Lincoln, stronger GEE (negative photosynthesis CO_2 contribution) gradually weakens the narrow CO_2 band immediately ahead of the cold front in the afternoon until it merges into the CO_2 background in the warm sector of the front (not shown).

The morning and noontime CO_2 band extends from the surface into the free troposphere (Fig. 10b, 11a) ahead of the cold front, which is related to nighttime convective transport of accumulated CO_2 from the nighttime stable boundary layer into the free troposphere (Fig. 14). The snapshots at 0200 CST shows significant updrafts and downdrafts ahead of the front associated with moist convection, which ejects the near-surface CO_2-rich and water vapor-rich air mass into the free troposphere. As a result, a weaker CO_2 band extends at least 3-4 km AGL (Fig. 11a). This may explain other CO_2 bands observed in the free troposphere by ACT-America flights. The moist convection in the region is more active during nighttime and weakens during the day on 4 August, which might be related to the diurnal variation of low-level jet (LLJ) over the Great Plains. On the night of 3-4 August, a strong LLJ is formed ahead of the cold front (not shown). The nighttime convection is presumably enhanced by convergence at the northern end of the LLJ over the

Northern Great Plains. Moist convective transport of chemical species has been reported to have significant impacts on air quality (Barth et al., 2007; Hu et al., 2010a; Jiang et al., 2007; Langford et al., 2010); it similarly impacts CO_2 transport and its budget in this case, as also shown by Penn State simulations.

3.2.2 Analysis of WRF-VPRM sensitivity simulations to examine cloud impacts

Clouds associated with moist convection block shortwave radiation during the day, thus affecting photosynthesis, and the land surface energy balance and eventually terrestrial CO_2 fluxes. Two sensitivity simulations (summarized in Table 2) are conducted to examine the impact of clouds on terrestrial fluxes and the frontal CO_2 band. In the clear-sky-photosynthesis simulation, clear-sky radiation is used to drive VPRM. The difference between clear-sky-photosynthesis and control runs shows the impact of clouds shading on terrestrial CO_2 fluxes (through Eq. 3), and subsequent impact on frontal CO_2 structures. During the night of 3-4 August, moist convection initially develops along the frontal boundary due to convergence. Through time, the convection lags behind the surface cold front convergence line along the southwest end of the convection line (Fig. 15). In the control simulation, reduced shortwave radiation due to cloud shading suppressed GEE, thus leading to enhanced biogenic CO_2. However, the enhanced biogenic CO_2 due to cloud shading (difference between control and clear-sky-photosynthesis) is minor (~2 ppm) comparing to the total enhancement in biogenic CO_2 ahead of the leading edge of the front (~20 ppm) and their position is not matching along the B200 flight track (Fig. 15). The storm weakens/shrinks from 10 to 12 CST and does not move while the surface front keeps moving southeastward (Fig. 16). So the biogenic CO_2 due to cloud shading at the time remains lagging behind the front while biogenic CO_2 during previous hours is transported southwesterly by the front, and the magnitude remains ~2 ppm (Fig. 16). Thus, cloud shading barely contributes to the CO_2 band ahead of the front observed by B200 in this case (Fig. 17).

At the northeast end of the convection line in the domain, the convection is at the leading edge of the front and the contribution from cloud shading to CO_2 concentration enhancement is more significant because biogenic activity is more vigorous (higher EVI), and convection is stronger in the region. Thus, in this region, cloud shading contributes more to the CO_2 band ahead of the front (Fig. 15, 16).

The impacts of clouds on CO_2 flux and mole fraction through the surface energy balance is more complex. Since the nested-domain WRF-VPRM simulations start at 0000 UTC 4 August (1800 CST), there is still daylight (shortwave radiation) in the first 2 hours of simulation during early evening. Using clear-sky shortwave radiation to drive surface energy balance in the clear-sky-surface-energy simulation initially leads to slightly higher temperature around clouds, which later on provides perturbation for the strong moist convection during nighttime (not shown), and the subsequent perturbation on CO_2 fields becomes quite non-linear, which can propagate through the rest of simulation. The deep moist convection weakens during the day and cloud shading on surface temperature becomes more linear. In the control simulation, cloud shading leads to lower surface temperature compared to the clear-sky-surface-energy simulation (Fig. 18g). Despite a nearly linear temperature response, its subsequent impact on CO_2 fluxes and mole fraction is complex. Compared to the clear-sky-surface-energy simulation, lower temperature in the control simulation results in lower respiration according to Eq. 4 and lower boundary layer height. Lower respiration leads to lower biogenic CO_2, but lower boundary layer on the other hand leads to more accumulation of respiration CO_2. The impact of lower surface temperature on photosynthesis is also mixed depending on whether the ambient temperature is lower or higher than the optimal temperature (T_{opt}) because optimal temperature leads to the strongest GEE through the highest T_{scale} (Mahadevan et al., 2008). In the morning of 4 August, temperature in the nested 4 km domain varies from 5°C to 35°C, spanning both sides of the T_{opt} (25 °C and 18 °C) of two dominant vegetation types in the domain, i.e., crop and grass. Thus, the impact of reduced temperature due to cloud shading on NEE is mixed (Fig. 18h). Another likely impact of lower temperature behind the cold front is to slightly enhance the front penetration, which might explain the negative CO_2 difference between control and clear-sky-surface-energy along some portion of the front. Thus, with all these impacts, CO_2 difference between the control and clear-sky-surface-energy simulation has mixed results with both positive and negative values (Fig. 18i). Given the relatively small magnitude of these CO_2 difference (< 4 ppm), the elevated CO_2 mole fraction band ahead of the front is not alleviated by the impact of clouds on surface energy balance (Fig. 17).

4. Conclusions and Discussion

An enhanced CO_2 mole fraction band was often observed immediately ahead of cold fronts during the Atmospheric Carbon and Transport (ACT)-America mission and its cause is undetermined (Pal et al., 2020). Improved understanding and correct simulation of these CO_2 bands are needed for unbiased inverse CO_2 flux estimation. Such CO_2 bands are hypothesized to be related to nighttime CO_2 respiration and investigated in this study using WRF-VPRM, an online-coupled weather-biosphere model. While the original version of VPRM is mechanistically realistic and satisfactorily parameterizes gross ecosystem exchange with appropriate calibration, its treatment for terrestrial respiration, a linear dependence on temperature only, is inadequate to simulate ecosystem respiration that is nonlinear and also depends on biomass and soil wetness. In this study, an improved terrestrial respiration parameterization that adds enhanced vegetation index (EVI), water stress scaling factor (W_{scale}) and its interactions with temperature to capture soil moisture effects, and a quadratic function of temperature (Gourdji et al., 2020) is incorporated into the WRF-coupled VPRM and evaluated first in a year-long dynamic downscaling simulation before being applied to investigate the CO_2 band ahead of a cold front on 4 August 2016.

The year-long downscaling simulation for 2016 is conducted over the contiguous United States at a 12 km grid spacing with spectral nudging to help maintain consistency of large scale flows with the driving reanalyses. Evaluations show that the improved WRF-VPRM simulates a stronger respiration (and stronger GEE also), thus showing a better skill to reproduce nighttime near-surface CO_2 peaks measured at six NOAA towers.

Nested-domain WRF-VPRM simulations including a 4-km inner domain covering the Northern Great Plains are conducted for 4 August 2016 to examine the CO_2 band formation mechanism. The control simulation is shown to be able to capture main characteristics of the CO_2 bands, albeit with certain biases in magnitudes and/or locations. Nighttime terrestrial respiration leads to accumulation of near-surface CO_2 in the region. As the cold front with low-CO_2 air mass moves southeastward, together with strong photosynthesis depleting CO_2 further southeast of the front, an enhanced CO_2 mole fraction band develops immediately ahead of the front. Two sensitivity simulations are conducted to examine the impact of cloud shading on CO_2 attributions, using clear-sky radiation (i.e., neglecting cloud effects on radiation parameterization) to drive VPRM and land surface energy balance respectively. Cloud shading is not found to enhance or alleviate the CO_2 band observed by the ACT-America flight in this case because the cloud shading-induced perturbation of biogenic CO_2 through radiative and surface temperature effects is not significant and its location lags behind the surface cold front.

Though not shown here, a few other CO_2 bands ahead of cold front including the ones on Oct 18, 2017, and May 2, 2018, were also examined using WRF-VPRM simulations. Nighttime accumulation of respiration CO_2 is found to contribute substantially to these CO_2 bands, as in the case of 4 August 2016 (Hu et al., 2020a).

Parameterization of impact of radiation on photosynthesis in VPRM through Eq. (3) may be overly simplified. Some studies reported enhanced photosynthesis in presence of diffuse radiation. Such a process is not currently considered in VPRM. Nonetheless, this study illustrates the first-order effect of cloud shading on terrestrial CO_2 fluxes and CO_2 attribution around cold fronts.

This study finds that respiration fluxes contribute significantly to the CO_2 bands ahead of cold fronts. Further improvement of terrestrial respiration parameterization, particularly over biologically-very-active land covers, is warranted to improve CO_2 simulations in the vicinity of mesoscale/synoptic weather systems, which is critical to accurately estimate regional CO_2 budgets (Chan et al., 2004; Pal et al., 2020). In addition, transport/dispersion, particularly during nighttime, could also be improved to reduce CO_2 biases (Hu et al., 2013).

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References are made to certain commercially available products in this paper to adequately specify the experimental procedures involved. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that these products are the best for the purpose specified.

The reanalysis data set was downloaded from https://rda.ucar.edu/, and the CT2017 data were provided by NOAA ESRL, Boulder, Colorado, USA from the website at http://carbontracker.noaa.gov. Tomohiro Oda provided the 0.1°×0.1° Open-Data Inventory for

Anthropogenic Carbon dioxide (ODIAC) emissions. *Monthly ocean CO_2 fluxes are downloaded from https://www.ldeo.columbia.edu/res/pi/CO2/carbondioxide/pages/air_sea_flux_2000.html. ACT-America data (DOI* 10.3334/ORNLDAAC/1593*) is downloaded from* https://doi.org/10.3334/ORNLDAAC/1593. AmeriFlux data are downloaded from *https://ameriflux.lbl.gov/sites/site-search/*
Model data produced from this study have been archived at the oasis data server at the San Diego Supercomputer Center, `/oasis/projects/nsf/uok114/xhu2/CO2_and_otherGHG`

Table 1. Parameter values used in this study. Units for parameters are as follows: λ: μmol CO_2 $m^{-2}s^{-1}$/μmol PAR $m^{-2}s^{-1}$; β, λ, γ, k_1: μmol CO_2 $m^{-2}s^{-1}$; PAR0: μmol PAR $m^{-2}s^{-1}$; α_1, k_2: μmol CO_2 $m^{-2}s^{-1}{}^{\circ}C^{-1}$; α_2, k_3: μmol CO_2 $m^{-2}s^{-1}{}^{\circ}C^{-2}$; temperature and the temperature parameters are in °C. Parameters for shrub and grass are specifically optimized for this study, but other parameters are taken from Gourdji et al (2020).

	Evergreen Forest	Deciduous Forest	Mixed forest	Shrub	Savanna	Crop	Grass
T_{crit}	1	13	2	12	11	-1	3
T_{scale2}	0.05	0.1	0.05	0	0.2	0.05	0.2
T_{min}	0	0	0	0	0	2	2
T_{opt}	20	20	20	20	20	25	18
T_{max}	40	40	40	40	40	40	40
PAR_0	477.3	594	453	320	722	2782	900
λ	-0.122	-0.096	-0.121	-0.074	-0.10	-0.078	-0.124
β	0.560	-14.048	0.077	0.922	-4.124	-0.156	-1.650
α_1	0.120	1.766	0.132	-0.114	0.68	0.072	0.180
α_2	0.003	-0.048	0.001	0.002	-0.018	-0.001	-0.006
γ	1.430	5.349	3.20	5.944	3.269	5.501	9.050
k_1	-0.531	9.008	-0.799	0.570	2.698	0.145	0.944
k_2	0.181	-1.207	0.182	-0.109	-0.382	-0.152	-0.260
k_3	-0.005	0.038	-0.002	0.004	0.016	0.016	0.013

Table 2. configurations for nested-domain sensitivity simulations

Simulations	configuration	Purpose
Control	fully coupled	to diagnose the formation mechanism of the CO_2 band ahead of the cold front
clear-sky-photosynthesis	use clear-sky radiation to drive VPRM	The difference between clear-sky-photosynthesis and control runs shows the impact of clouds shading on terrestrial CO_2 fluxes, and subsequent impact on frontal CO_2 structures
clear-sky-surface-energy	use clear-sky radiation to drive the Noah land surface model	The difference between clear-sky-surface-energy and control runs shows the impact of clouds on surface energy balance, and subsequent impact on frontal CO_2 structures

Table 3. Overall statistics for simulated CO_2 over six NOAA towers during both daytime and nighttime by WRF-VPRM_G in this study and WRF-VPRM in Hu et al. (2020b).

The metrics include correlation coefficient r, mean bias (MB), mean absolute gross error (MAGE), root mean-square error (RMSE), and normalized mean bias (NMB). Their formula can be found in Seigneur et al. (2000).

	day and night											
Sites	AMT		BAO		LEF		SCT		WBI		WKT	
Simulations	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM
Mean obs, ppm	415.12	415.12	417.12	417.12	411.33	411.33	416.47	416.47	416.19	416.19	414.32	414.32
Mean sim, ppm	410.84	406.16	414.72	412.66	410.05	405.63	417.67	414.42	415.42	409.39	415.59	410.72
Number	8153	8153	4742	4742	8124	8124	7940	7940	7754	7754	8024	8024
r	0.52	0.34	0.51	0.45	0.65	0.57	0.75	0.71	0.63	0.46	0.71	0.57
MB, ppm	-4.28	-8.96	-2.39	-4.45	-1.29	-5.70	1.20	-2.05	-0.77	-6.80	1.27	-3.61
MAGE, ppm	7.91	10.19	6.89	7.41	5.31	6.77	5.84	6.07	7.04	8.81	5.07	5.74
RMSE, ppm	15.54	19.00	10.84	11.80	9.05	11.52	8.03	8.74	11.58	15.48	7.01	8.84
NMB, %	-1.0	-2.2	-0.6	-1.1	-0.3	-1.4	0.3	-0.5	-0.2	-1.6	0.3	-0.9

Table 4. Evaluation statistics for simulated CO_2 over six NOAA towers during daytime between 10-18 CST.

	late day (10-18CST)											
Sites	AMT		BAO		LEF		SCT		WBI		WKT	
Simulations	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM
Mean obs, ppm	405.57	405.57	412.52	412.52	405.62	405.62	407.39	407.39	408.43	408.43	408.25	408.25
Mean sim, ppm	406.5	403.43	410.96	410.3	407.36	403.98	410.57	408.4	411.04	406.81	410.95	408.44
Number	2836	2836	1642	1642	2826	2826	2771	2771	2676	2676	2782	2782
r	0.86	0.84	0.51	0.46	0.90	0.91	0.75	0.75	0.86	0.86	0.78	0.76
MB, ppm	0.92	-2.15	-1.56	-2.23	1.74	-1.64	3.19	1.02	2.61	-1.62	2.70	0.19
MAGE, ppm	3.98	4.28	5.62	5.88	3.68	3.48	4.86	4.13	5.32	4.85	4.14	3.28
RMSE, ppm	5.75	6.4	10.41	10.84	5.22	5.11	6.52	5.70	7.38	7.19	5.44	4.56
NMB, %	0.2	-0.5	-0.4	-0.5	0.4	-0.4	0.8	0.2	0.6	-0.4	0.7	0

Table 5. Evaluation statistics for simulated CO_2 over six NOAA towers during nighttime between 22-06 CST.

	late night (22-06CST)											
Sites	AMT		BAO		LEF		SCT		WBI		WKT	
Simulations	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM	VPRM_G	VPRM
Mean obs, ppm	424.99	424.99	421.1	421.1	416.99	416.99	424.73	424.73	423.13	423.13	419.43	419.43
Mean sim, ppm	414.62	408.58	417.85	414.65	412.58	407.26	423.64	419.52	418.95	411.67	419.22	412.53
Number	3197	3197	1865	1865	3182	3182	3100	3100	3055	3055	3152	3152
r	0.21	-0.12	0.39	0.34	0.24	0.11	0.57	0.50	0.31	-0.02	0.53	0.32
MB, ppm	-10.38	-16.42	-3.25	-6.45	-4.41	-9.72	-1.08	-5.20	-4.19	-11.46	-0.21	-6.9
MAGE, ppm	12.69	16.88	7.93	8.81	7.10	10.16	6.52	7.82	8.86	12.50	5.75	8.06
RMSE, ppm	22.79	27.79	11.29	12.79	12.02	15.91	9.10	10.89	14.67	20.66	8.11	11.54
NMB, %	-2.4	-3.9	-0.8	-1.5	-1.1	-2.3	-0.3	-1.2	-1.	-2.7	0	-1.6

Figure captions:

Figure 1. (a) enhanced vegetation index (EVI) on 4 August 2016, and (b) dominant vegetation types including water, evergreen forest, deciduous forest, mixed forest, shrubland, savanna, cropland, grassland, and urban derived from MODIS data in the simulation domain. The second domain with a 4 km grid spacing over the Northern Great Plains is marked. Six NOAA tower sites (LEF [WI], AMT [ME], WBI [IA], SCT [SC], BAO [CO], and WKT [TX]) are marked with hollow diamonds. The ACT-America B200 flight track is also marked. (c) MODIS cloud image on this day overlaid with OCO-2 XCO_2 observation.

Figure 2. Evaluation of (a,b) hourly CO_2 flux and (c,d) its median diurnal variation during growing season simulated by (left) VPRM with respiration parametrization using eq. (2) (Mahadevan et al., 2008) and (right) VPRM_G using eq. (4) (Gourdji et al., 2020) comparing to the NEE measurements at US-Ne3, a crop site. Growing season mean bias (MB) of day and nighttime fluxes are marked in (a) and (b).

Figure 3. Near-surface CO_2 in 2016, observed at six NOAA tower sites and simulated by WRF-VPRM_G. Note that CO_2 is measured at different heights AGL at different towers, simulated values are extracted at the corresponding model height. Nighttime and daytime mean bias (MB) of CO_2 at each site is marked.

Figure 4. Median diurnal variation of near-surface CO_2 during growing season (June-September) in 2016, observed at six NOAA tower sites and simulated by WRF-VPRM_G. Note that CO_2 is measured at different heights AGL at different towers, simulated values are extracted at the corresponding model height.

Figure 5. Near-surface CO_2 in first half of July 2016 (growing season for most sites), observed at six NOAA tower sites and simulated by WRF-VPRM_G in this study and WRF-VPRM in Hu et al. (2020b). Nighttime is shaded.

Figure 6. Mean CO_2 profiles in growing season (June-September) of 2016 (1st row) observed at (left) LEF and (right) AMT NOAA towers and simulated by (2nd row) WRF-VPRM_G in this study and (3rd row) WRF-VPRM in Hu et al. (2020b).

Figure 7. same as Figure 5, but at (left) WBI and (right) SCT NOAA towers.

Figure 8. same as Figure 5, but at (left) BAO and (right) WKT NOAA towers.

Figure 9. (1st row) Profiles of CO_2, potential temperature (θ), and water vapor mixing ratio simulated at 1000 CST and observed during the C130 ascending time between 1000-1015 CST on August 4 over the Lincoln airport (40.8367°N, 96.7619°W), and profiles of (left to right) wind speed, θ, and water vapor mixing ratio at 0600 CST on August 4 simulated and observed at sounding sites: (2nd-4th rows) KLBF, KOAX, and KTOP, which are marked on Fig. 10.

Figure 10. (a,c) horizontal (at ~995m above sea level) and (b,d) vertical cross sections of (left) CO_2 and (right) equivalent potential temperature (θ_e) through the B200 flight track at 1200 CST on August 4 simulated by WRF-VPRM_G, overlaid with B200 aircraft CO_2 data. Note that the flight path and CO_2 data are marked in panel a. The CST time is marked along the flight path.

Figure 11. (a) vertical cross sections of total CO_2 through the B200 flight track at 1200 CST on August 4 simulated by WRF-VPRM_G in the nested inner domain, overlaid with B200 aircraft CO_2 data and (b-f) CO_2 components including background, biogenic, anthropogenic, respiration, and photosynthesis CO_2. Location of Lincoln is marked using a star on X-Axis.

Figure 12. (a) Total CO_2 through the B200 flight track at 1200 CST on August 4 in the nested inner domain simulated by WRF-VPRM_G and WRF-VPRM, along with B200 aircraft CO_2 data in the boundary layer during 11:20-13:10 CST and (b-f) simulated CO_2 components including background, biogenic, anthropogenic, respiration, and photosynthesis CO_2. Location of Lincoln is marked using a star on X-Axis.

Figure 13. (top to bottom) Surface biogenic CO_2, respiration, and photosynthesis CO_2 at (a,b,c) 08 and (d,e,f) 12 CST. B200 aircraft CO_2 data in the boundary layer is overlaid for location reference.

Figure 14. (a) vertical cross sections of total CO_2 through the B200 flight track at 0200 CST on August 4 simulated by WRF-VPRM_G in the nested inner domain, overlaid with B200 aircraft CO_2 data and (b-d) CO_2 components including background, biogenic, anthropogenic CO_2, (e-f) vertical velocity, and hydrometer mixing ratio.

Figure 15. (top to bottom) surface short wave radiation, GEE, and biogenic CO_2 simulated by (left) control and (middle) the clear-sky-photosynthesis sensitivity simulation, and (right) their difference at 10 CST. B200 aircraft CO_2 data in the boundary layer at ~12 CST is overlaid.

Figure 16. difference of (top to bottom) surface short wave radiation, GEE, and biogenic CO_2 simulated by the control and the clear-sky-photosynthesis sensitivity simulation, at (left) 11 CST and (right) 12 CST. B200 aircraft CO_2 data in the boundary layer at ~12 CST is overlaid.

Figure 17. same as Figure 12, but simulated by the Sensitivity1 (clear-sky-photosynthesis) and Sensitivity2 (clear-sky-surface-energy) simulations.

Figure 18. (top to bottom) temperature at 2 m AGL (T2), NEE, and biogenic CO_2 simulated by (left) control and (middle) the clear-sky-surface-energy sensitivity simulation, and (right) their difference at 10 CST. B200 aircraft CO_2 data in the boundary layer at ~12 CST is overlaid.

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Figures.

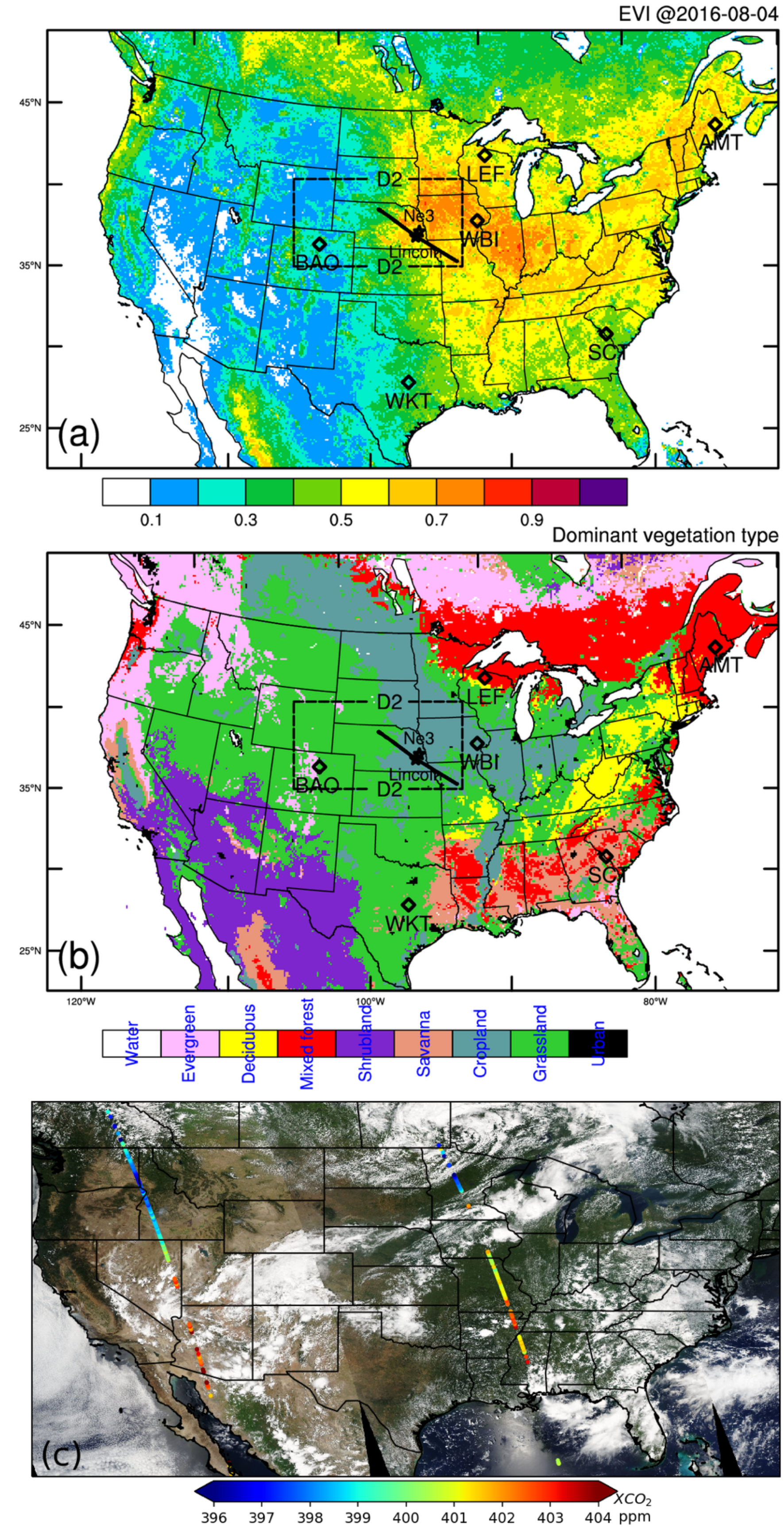
EVI @2016-08-04
45°N
35°N
25°N
(a)
AMT
LEF
D2
Ne3
WBI
Lincoln
BAO
SCT
WKT
0.1
0.3
0.5
0.7
0.9
Dominant vegetation type
(b)
120°W
100°W
80°W
Water
Evergreen
Deciduous
Mixed forest
Shrubland
Savanna
Cropland
Grassland
Urban
(c)
396
397
398
399
400
401
402
403
404
XCO_2
ppm

Figure 1. (a) enhanced vegetation index (EVI) on 4 August 2016, and (b) dominant vegetation types including water, evergreen forest, deciduous forest, mixed forest, shrubland, savanna, cropland, grassland, and urban derived from MODIS data in the simulation domain. The second domain with a 4 km grid spacing over the Northern Great Plains is marked. Six NOAA tower sites (LEF [WI], AMT [ME], WBI [IA], SCT [SC], BAO [CO], and WKT [TX]) are marked with hollow diamonds. The ACT-America B200 flight track is also marked. (c) MODIS cloud image on this day overlaid with OCO-2 XCO_2 observation.

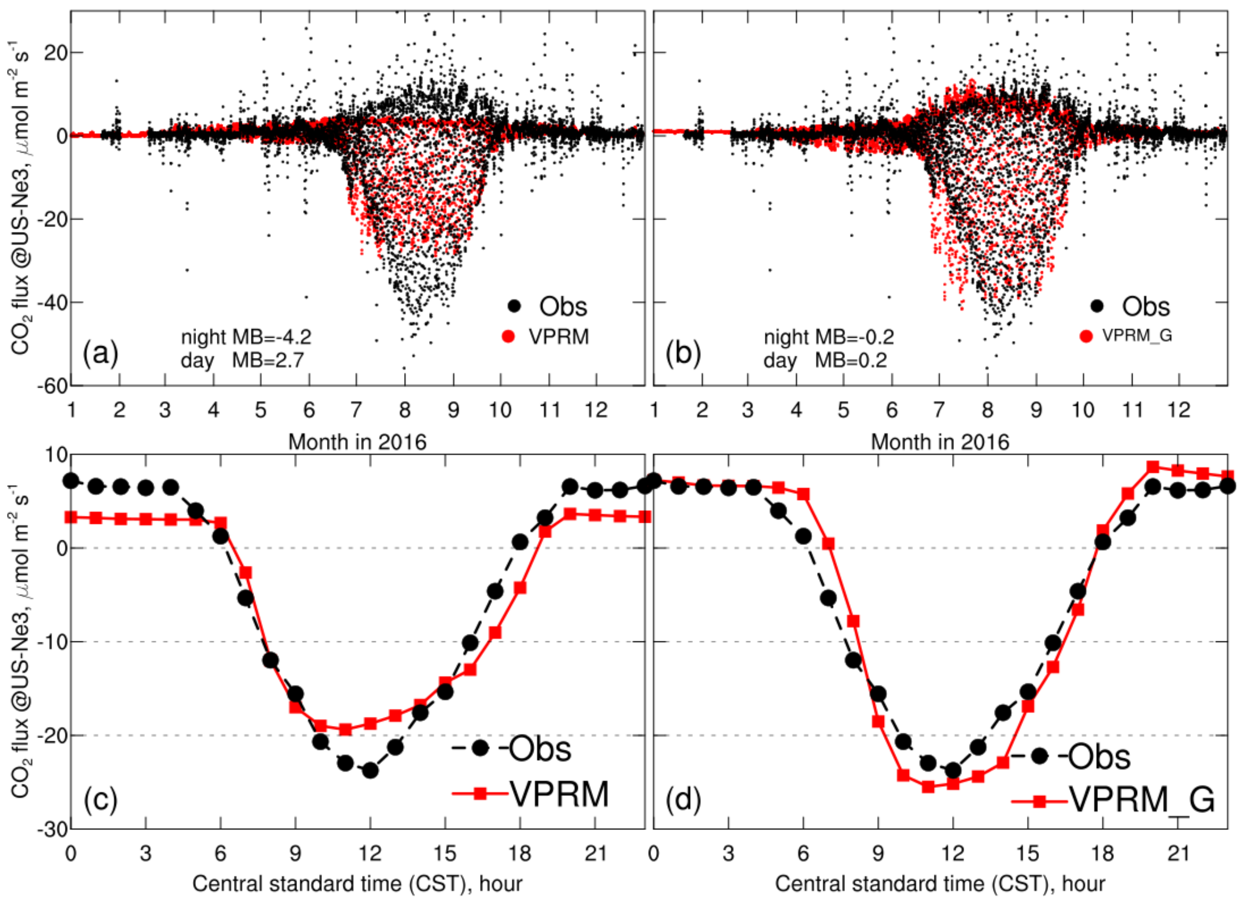

Figure 2. Evaluation of (a,b) hourly CO_2 flux and (c,d) its median diurnal variation during growing season simulated by (left) VPRM with respiration parametrization using eq. (2) (Mahadevan et al., 2008) and (right) VPRM_G using eq. (4) (Gourdji et al., 2020) comparing to the NEE measurements at US-Ne3, a crop site. Growing season mean bias (MB) of day and nighttime fluxes are marked in (a) and (b).

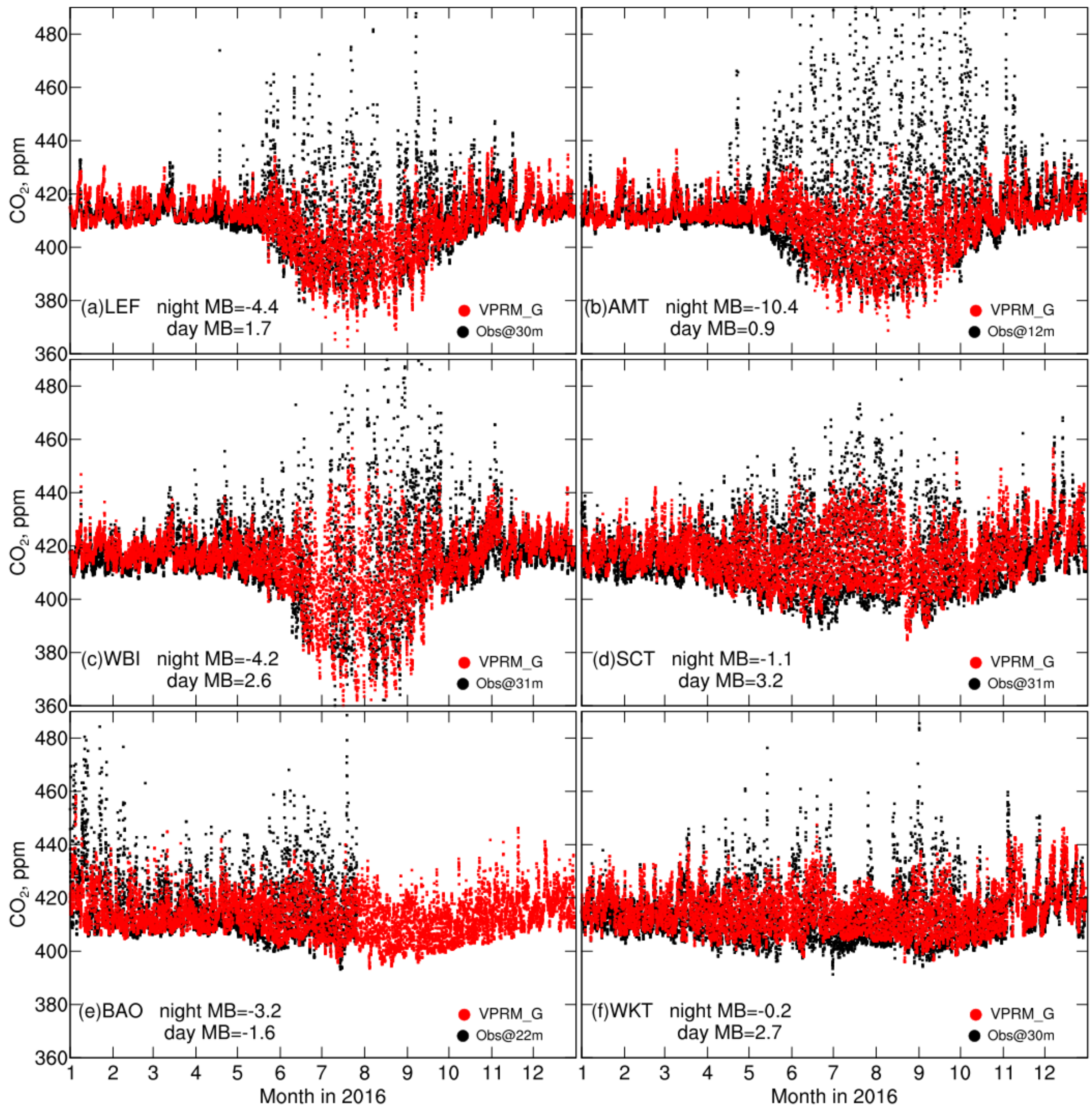

Figure 3. Near-surface CO_2 in 2016, observed at six NOAA tower sites and simulated by WRF-VPRM_G. Note that CO_2 is measured at different heights AGL at different towers, simulated values are extracted at the corresponding model height. Nighttime and daytime mean bias (MB) of CO_2 at each site is marked.

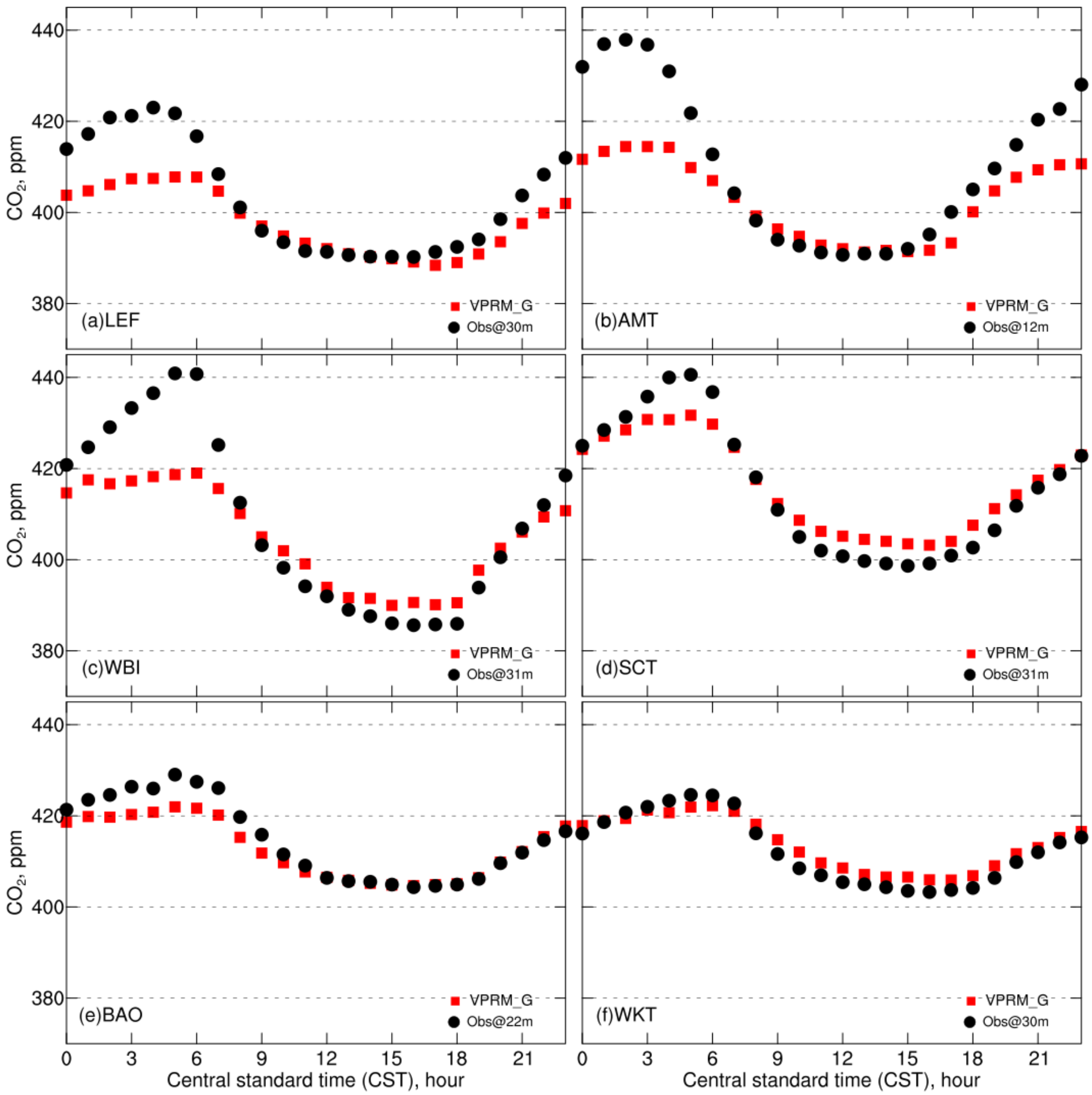

Figure 4. Median diurnal variation of near-surface CO_2 during growing season (June-September) in 2016, observed at six NOAA tower sites and simulated by WRF-VPRM_G. Note that CO_2 is measured at different heights AGL at different towers, simulated values are extracted at the corresponding model height.

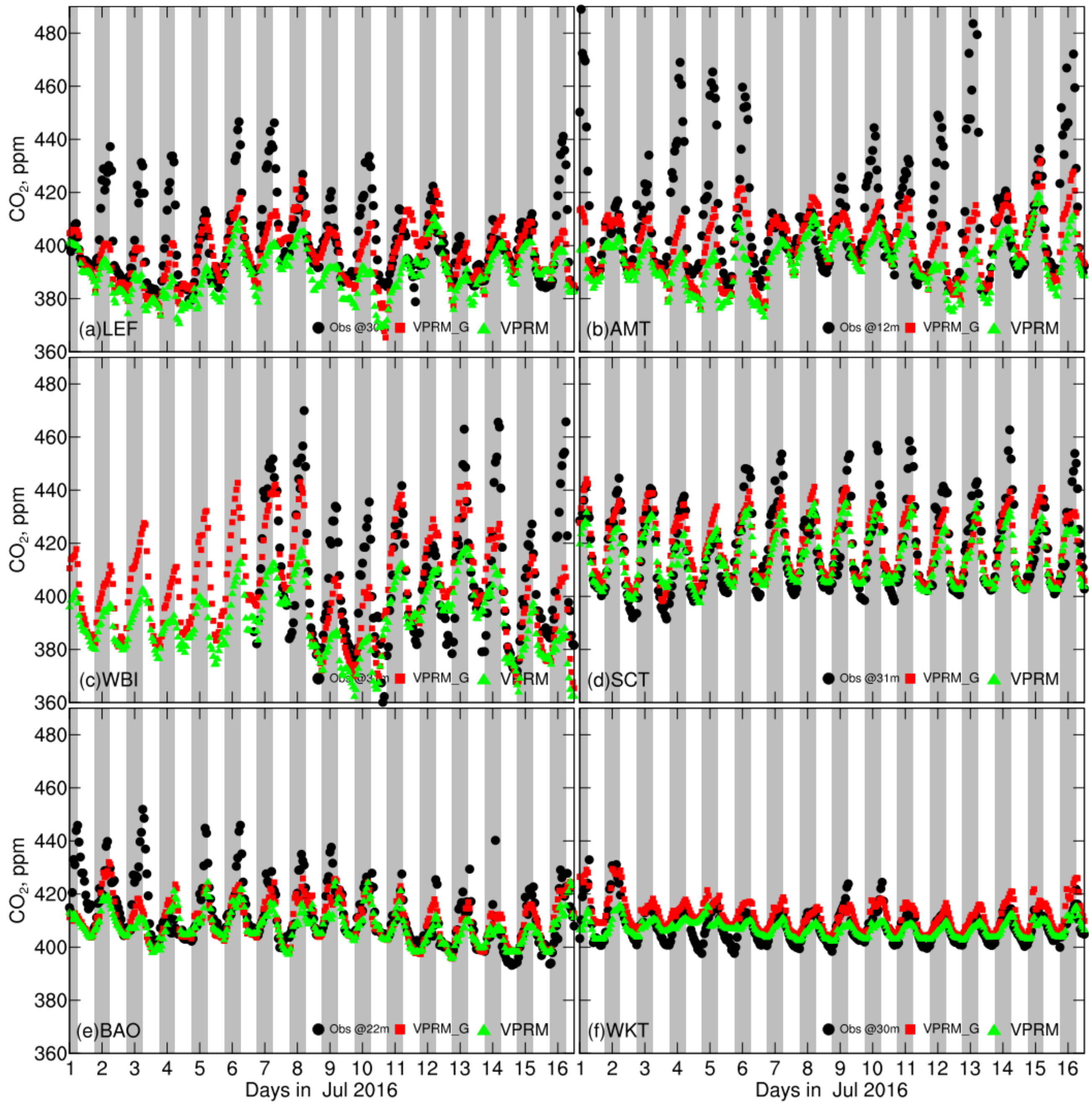

Figure 5. Near-surface CO_2 in first half of July 2016 (growing season for most sites), observed at six NOAA tower sites and simulated by WRF-VPRM_G in this study and WRF-VPRM in Hu et al. (2020). Nighttime is shaded.

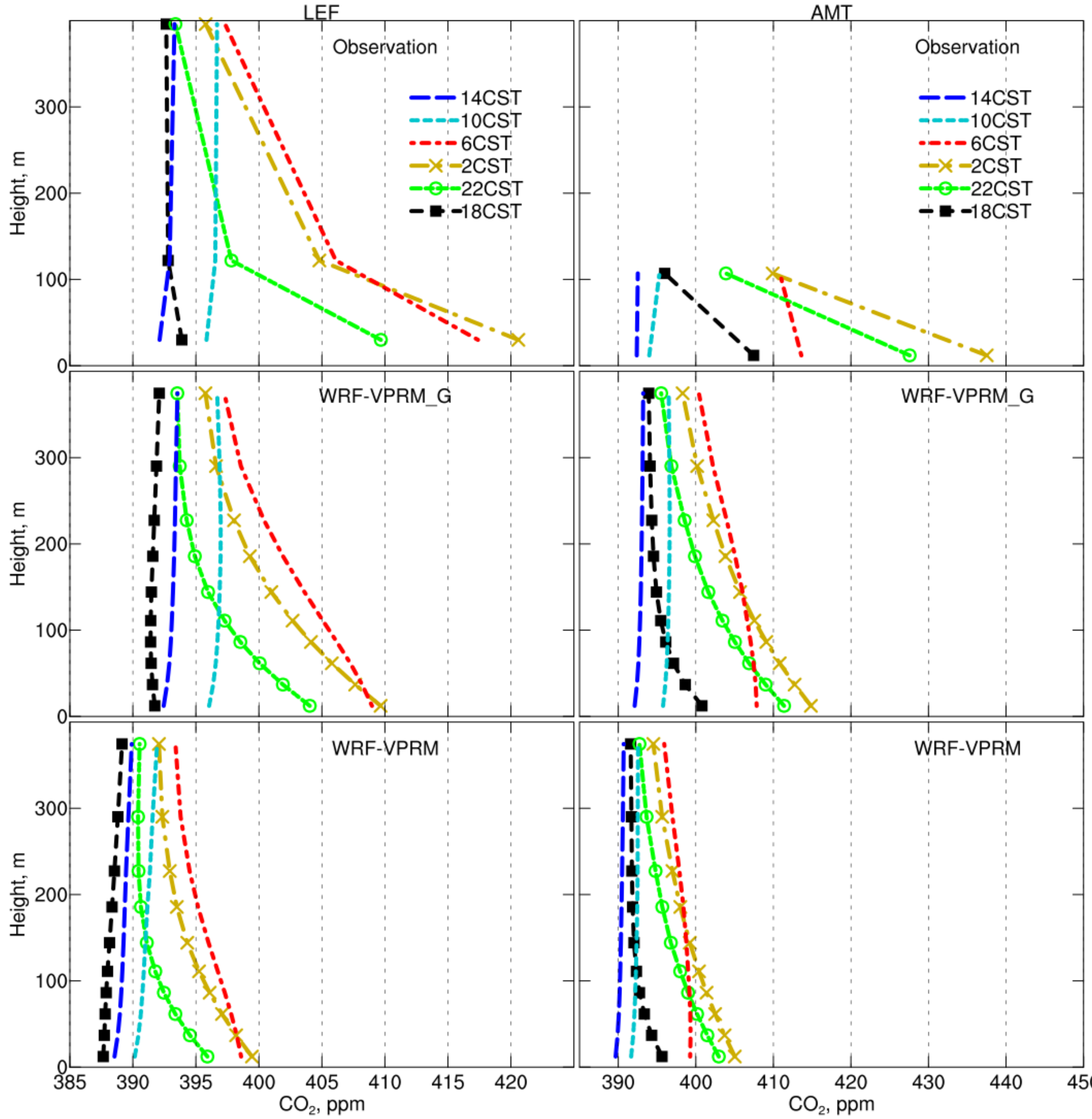

Figure 6. Mean CO_2 profiles in growing season (June-September) of 2016 (1st row) observed at (left) LEF and (right) AMT NOAA towers and simulated by (2nd row) WRF-VPRM_G in this study and (3rd row) WRF-VPRM in Hu et al. (2020).

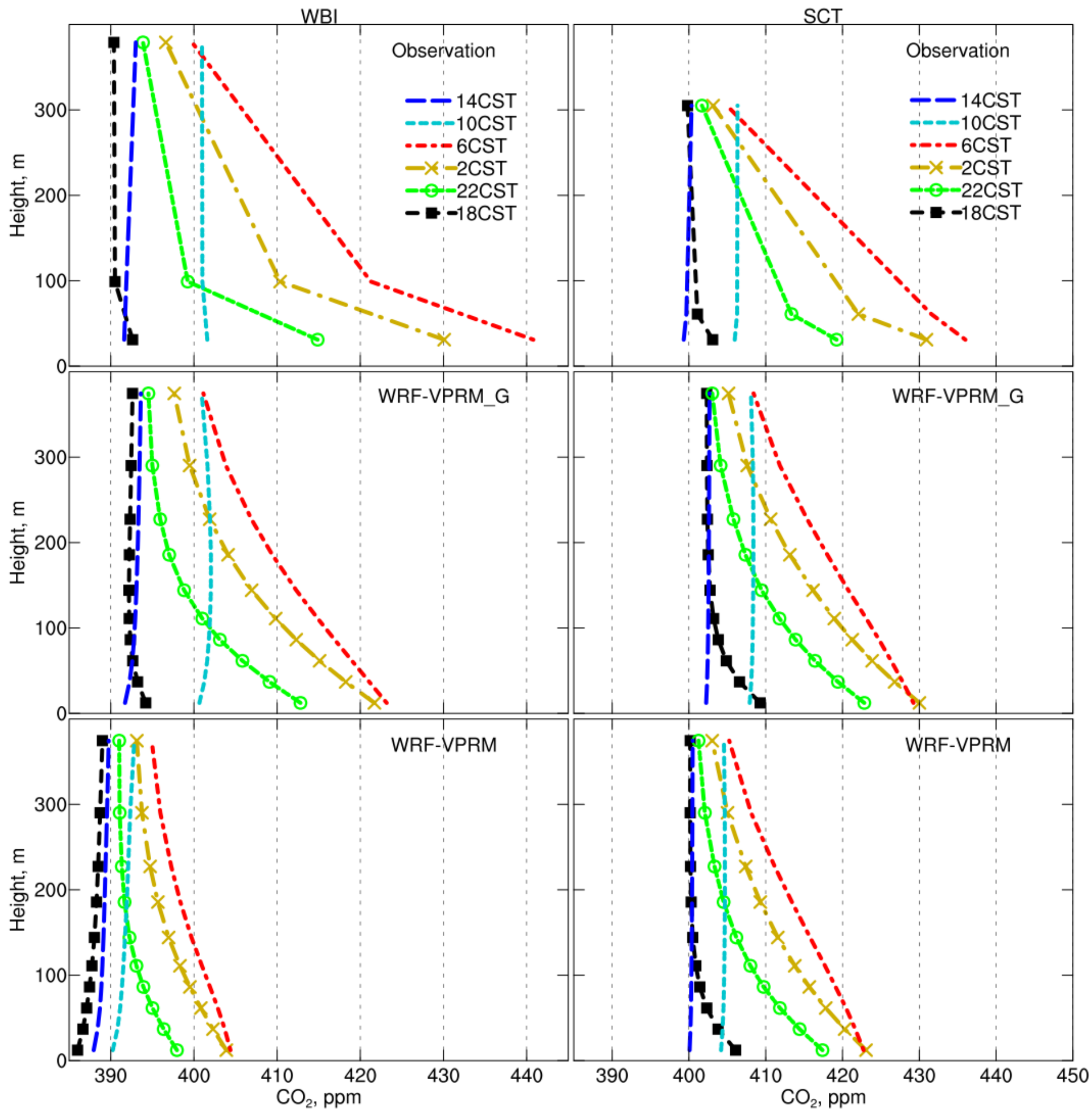

Figure 7. same as Figure 6, but at (left) WBI and (right) SCT NOAA towers.

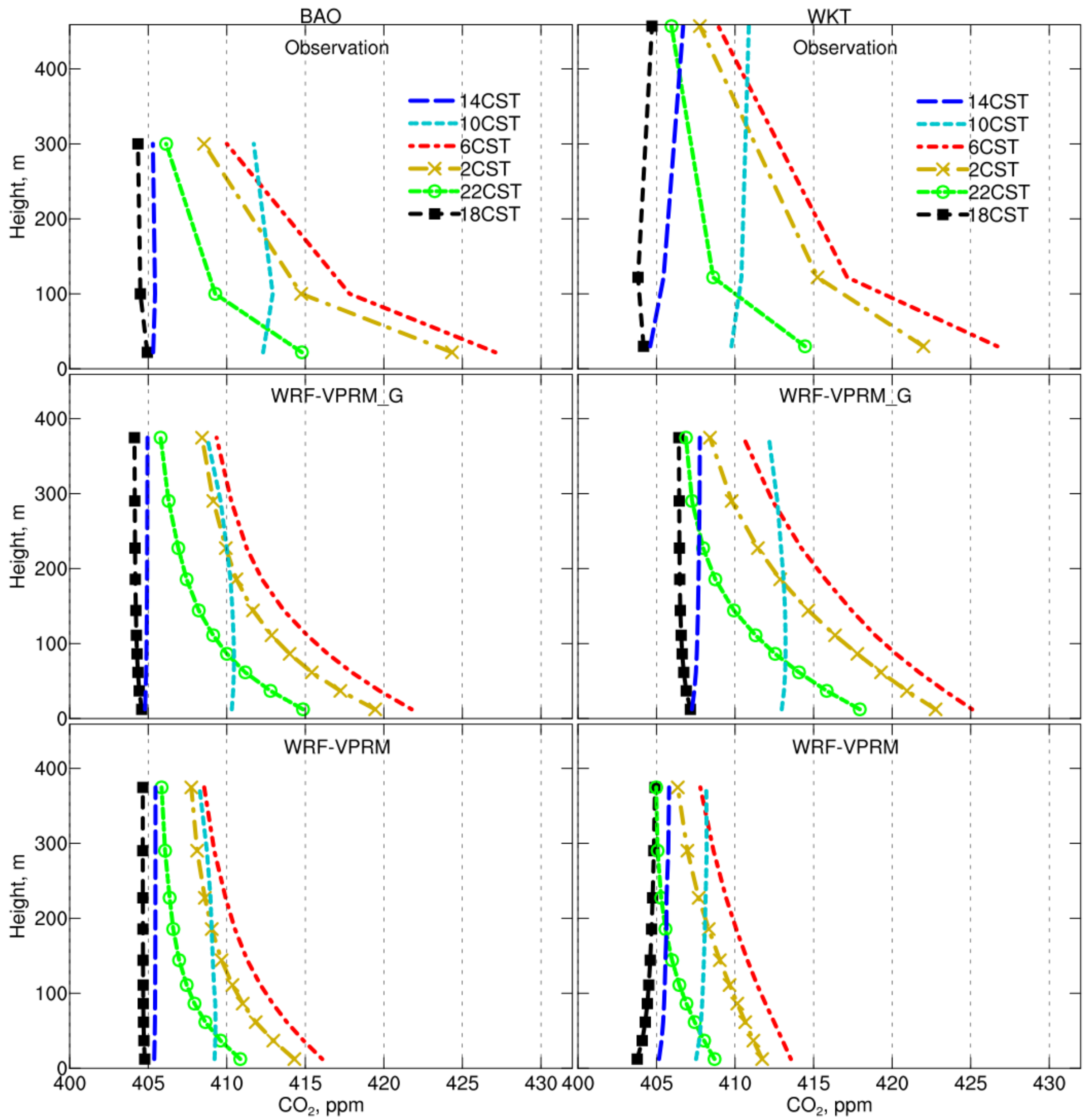

Figure 8. same as Figure 6, but at (left) BAO and (right) WKT NOAA towers.

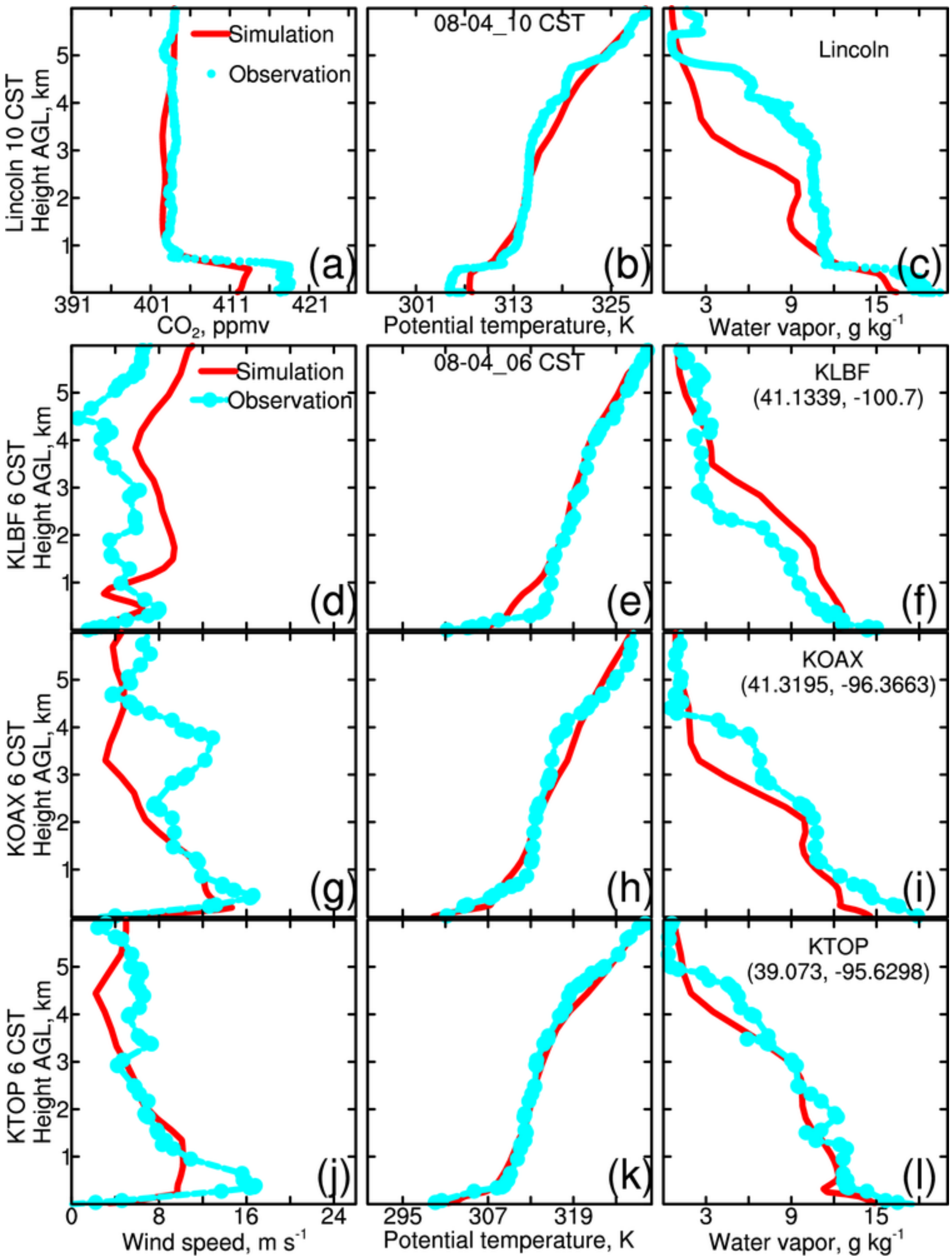

Figure 9. (1st row) Profiles of CO_2, potential temperature (θ), and water vapor mixing ratio simulated at 1000 CST and observed during the C130 ascending time between 1000-1015 CST on August 4 over the Lincoln airport (40.8367°N, 96.7619°W), and profiles of (left to right) wind speed, θ, and water vapor mixing ratio at 0600 CST on August 4 simulated and observed at sounding sites: (2nd-4th rows) KLBF, KOAX, and KTOP, which are marked on Fig. 10.

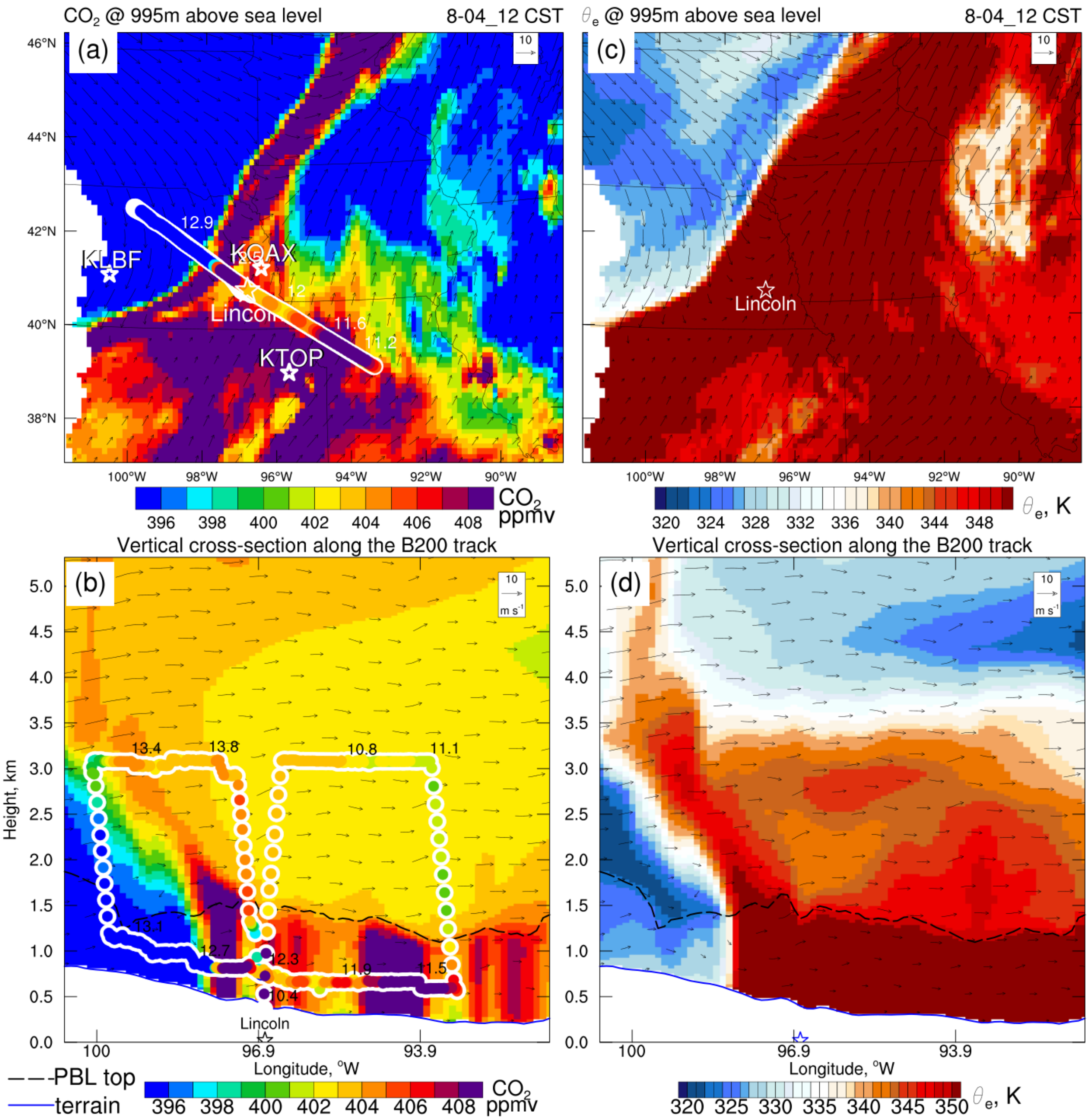

Figure 10. (a,c) horizontal (at ~995m above sea level) and (b,d) vertical cross sections of (left) CO_2 and (right) equivalent potential temperature (θ_e) through the B200 flight track at 1200 CST on August 4 simulated by WRF-VPRM_G, overlaid with B200 aircraft CO_2 data. Note that the flight path and CO_2 data are marked in panel a. The CST time is marked along the flight path.

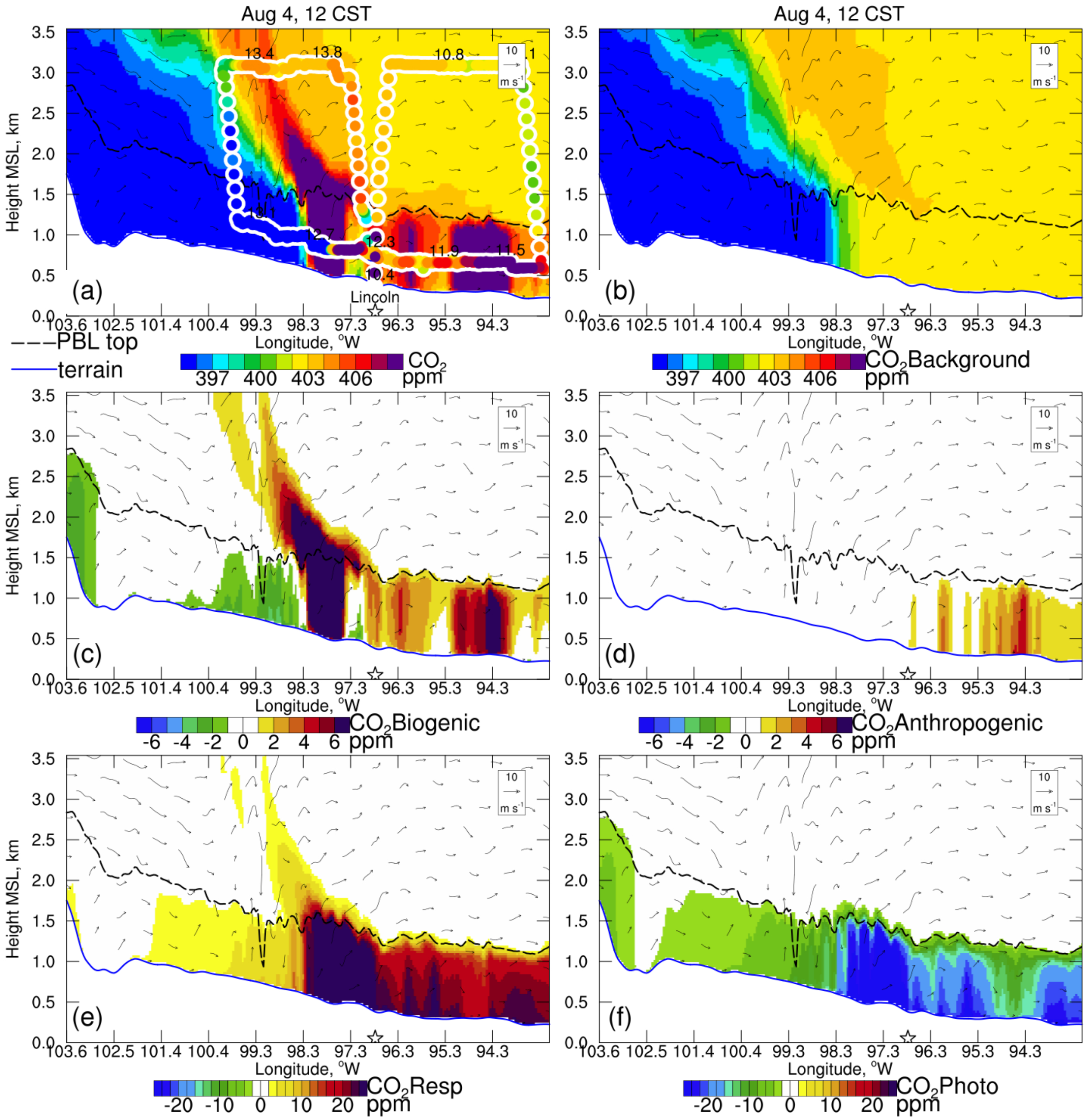

Figure 11. (a) vertical cross sections of total CO_2 through the B200 flight track at 1200 CST on August 4 simulated by WRF-VPRM_G in the nested inner domain, overlaid with B200 aircraft CO_2 data and (b-f) CO_2 components including background, biogenic, anthropogenic, respiration, and photosynthesis CO_2. Location of Lincoln is marked using a star on X-Axis.

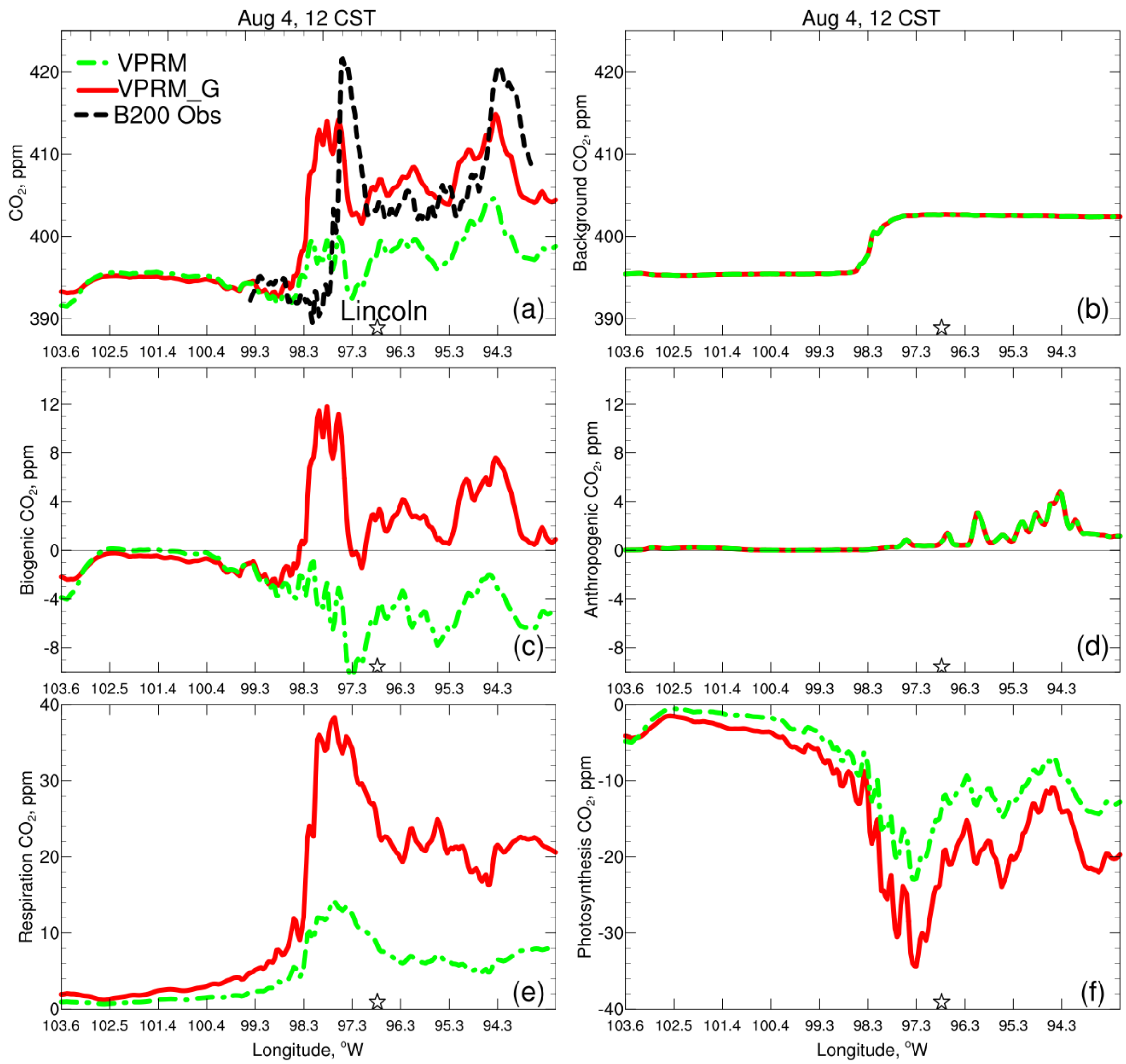

Figure 12. (a) Total CO_2 through the B200 flight track at 1200 CST on August 4 in the nested inner domain simulated by WRF-VPRM_G in this study and WRF-VPRM in Hu et al. (2020), along with B200 aircraft CO_2 data in the boundary layer during 11:20-13:10 CST and (b-f) simulated CO_2 components including background, biogenic, anthropogenic, respiration, and photosynthesis CO_2. Location of Lincoln is marked using a star on X-Axis.

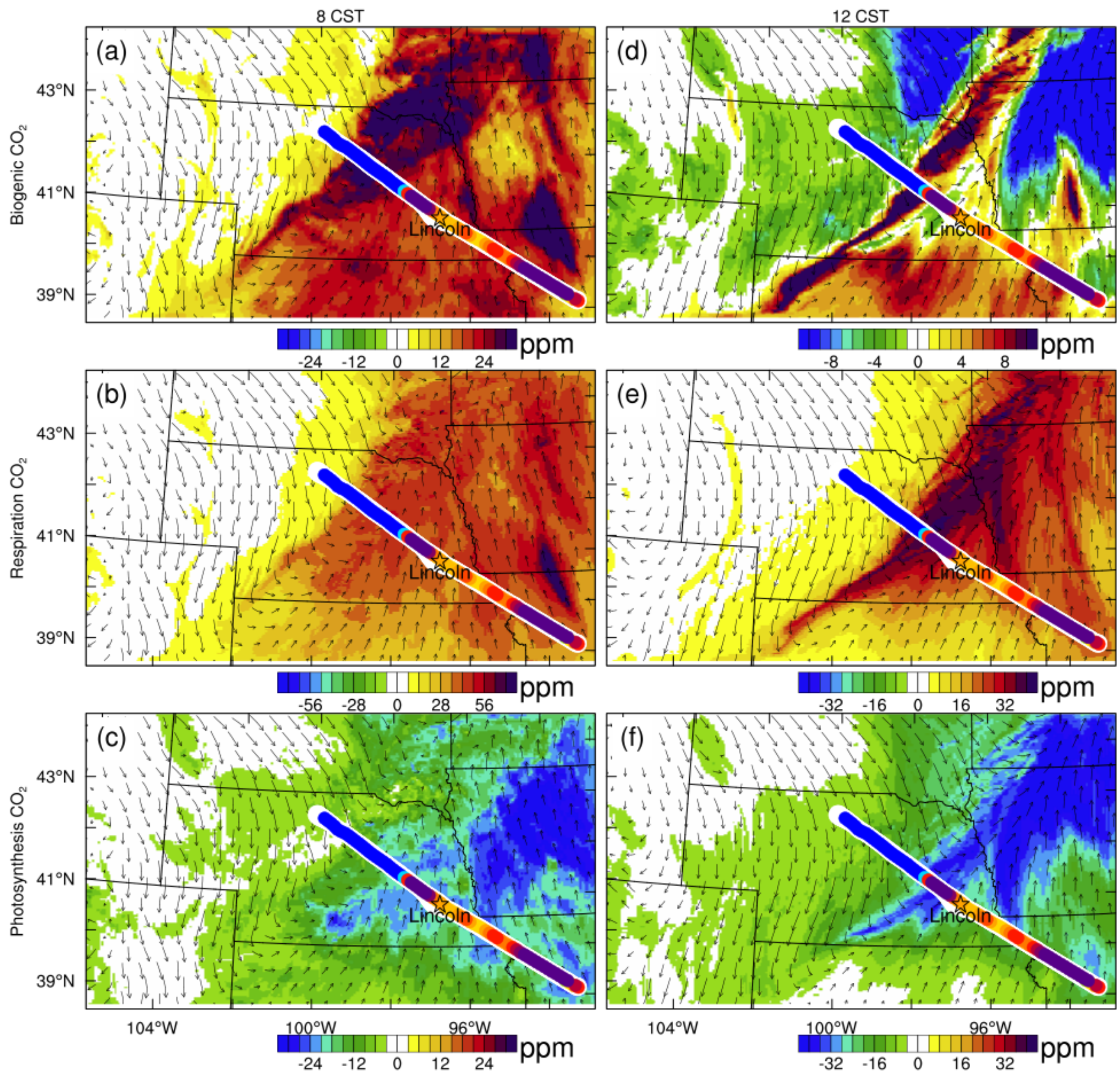

Figure 13. (top to bottom) Surface biogenic CO_2, respiration, and photosynthesis CO_2 at (a,b,c) 08 and (d,e,f) 12 CST. B200 aircraft CO_2 data in the boundary layer is overlaid for location reference.

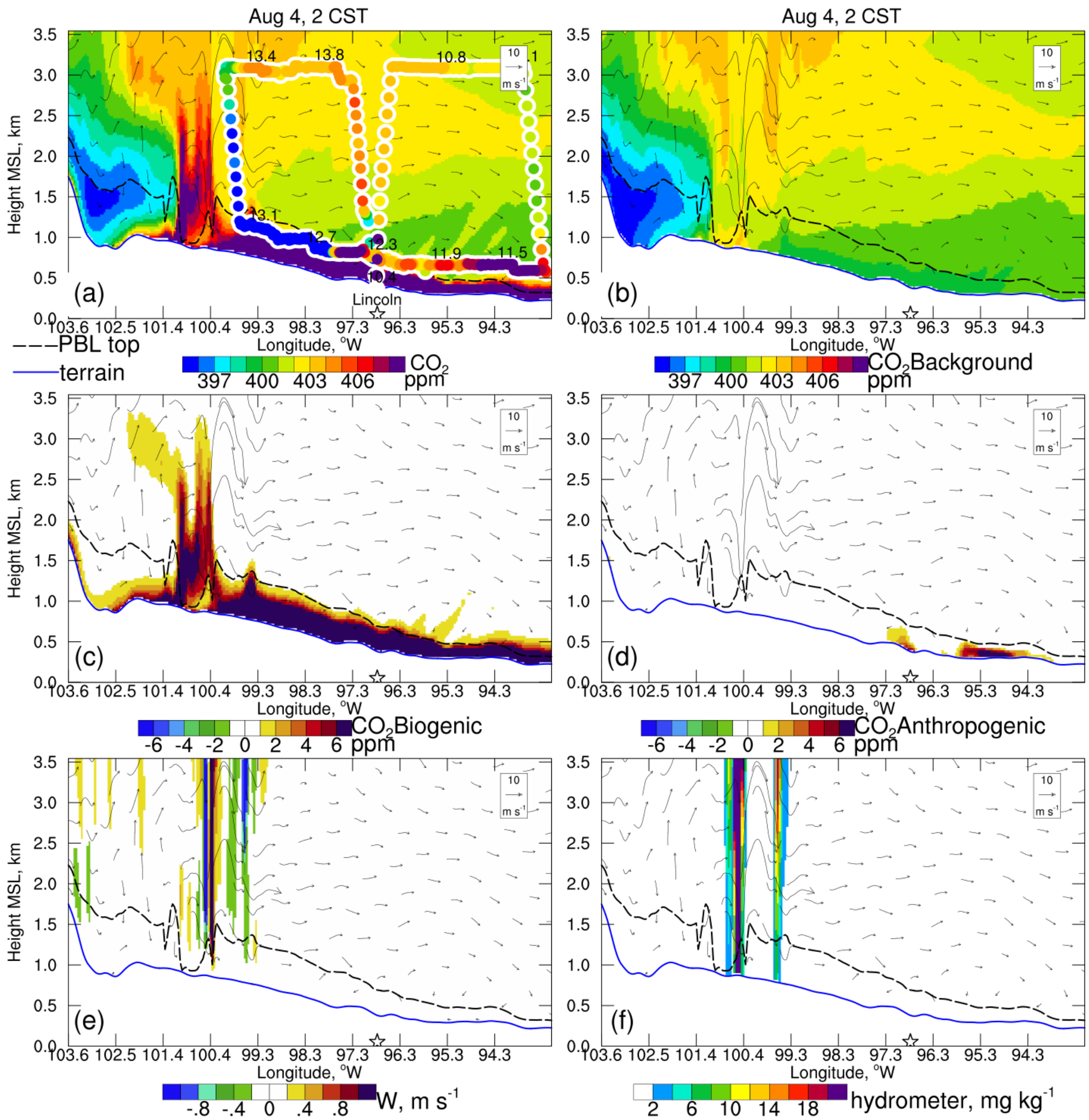

Figure 14. (a) vertical cross sections of total CO_2 through the B200 flight track at 0200 CST on August 4 simulated by WRF-VPRM_G in the nested inner domain, overlaid with B200 aircraft CO_2 data and (b-d) CO_2 components including background, biogenic, anthropogenic CO_2, (e-f) vertical velocity, and hydrometer mixing ratio.

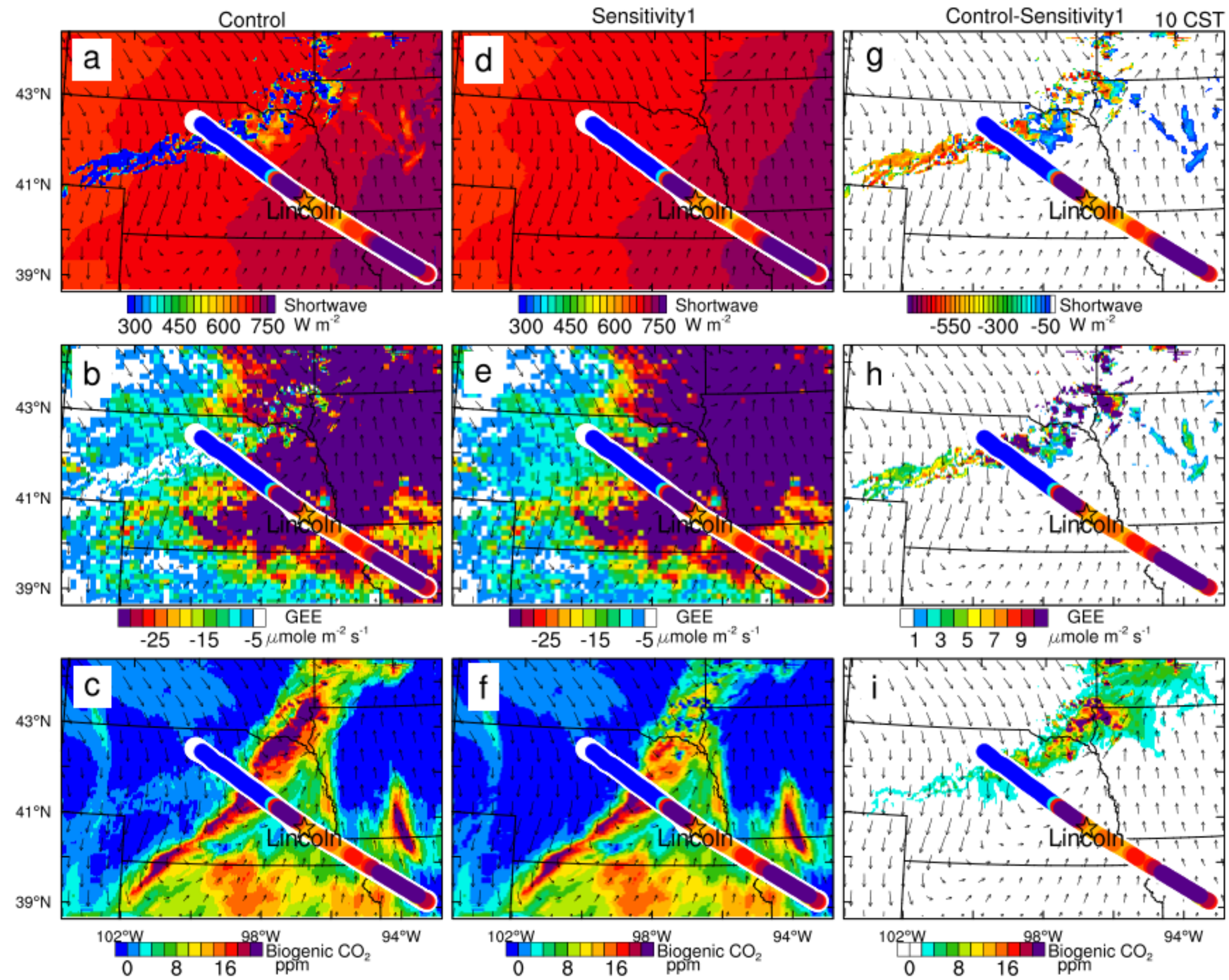

Figure 15. (top to bottom) surface short wave radiation, GEE, and biogenic CO_2 simulated by (left) control and (middle) the clear-sky-photosynthesis sensitivity simulation, and (right) their difference at 10 CST. B200 aircraft CO_2 data in the boundary layer at ~12 CST is overlaid.

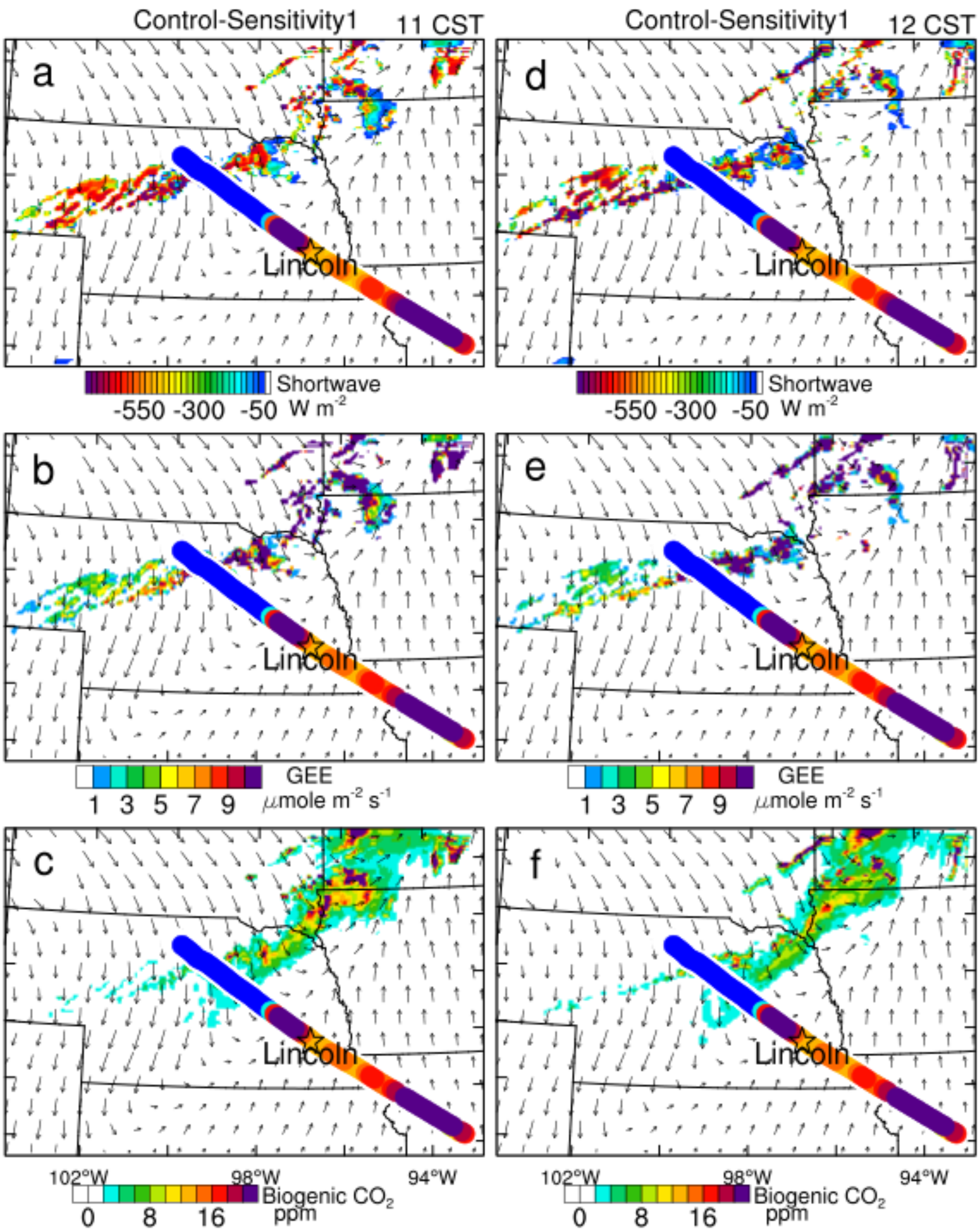

Figure 16. difference of (top to bottom) surface short wave radiation, GEE, and biogenic CO_2 simulated by the control and the clear-sky-photosynthesis sensitivity simulation, at (left) 11 CST and (right) 12 CST. B200 aircraft CO_2 data in the boundary layer at ~12 CST is overlaid.

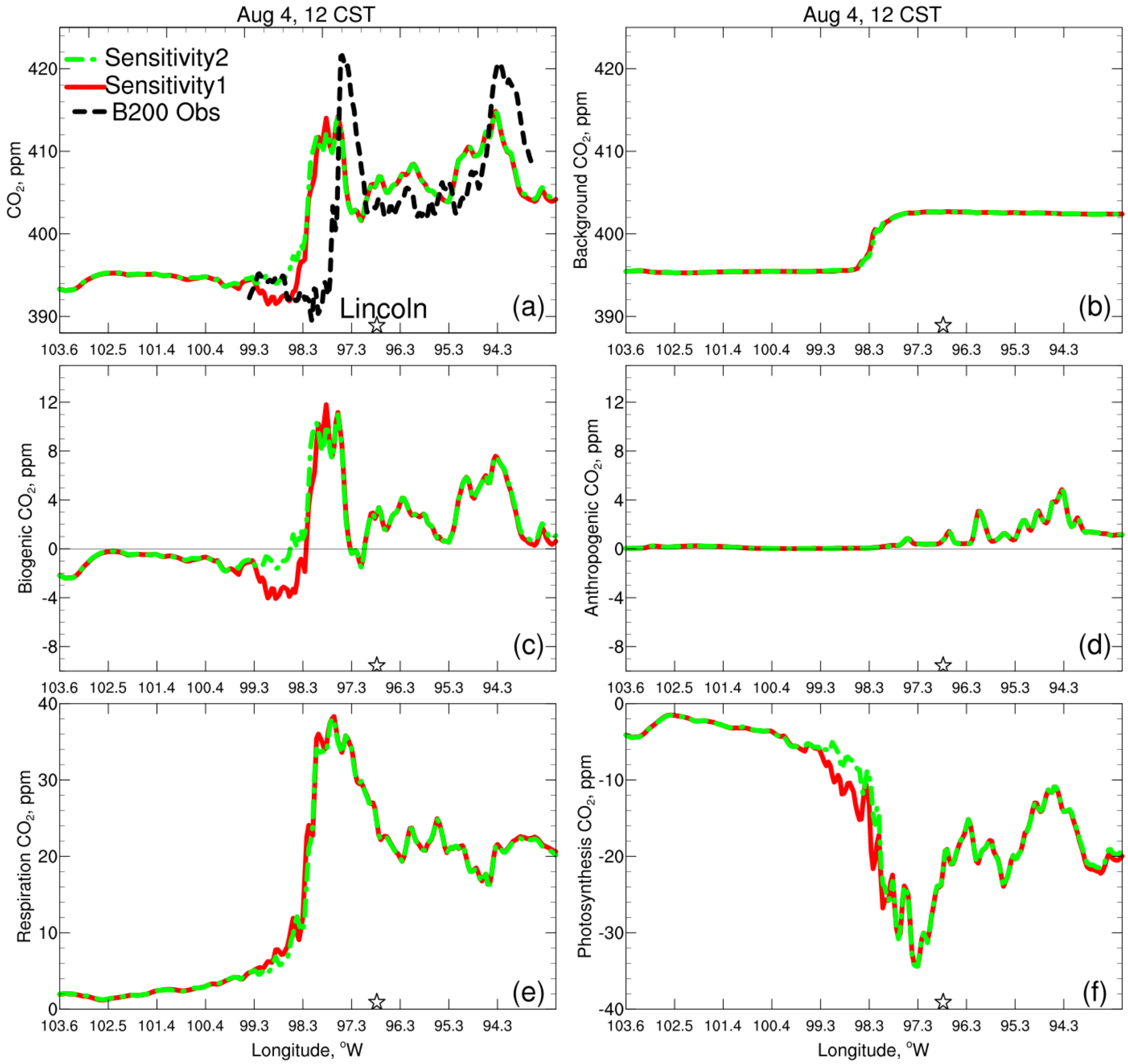

Figure 17. same as Figure 12, but simulated by the Sensitivity1 (clear-sky-photosynthesis) and Sensitivity2 (clear-sky-surface-energy) simulations.

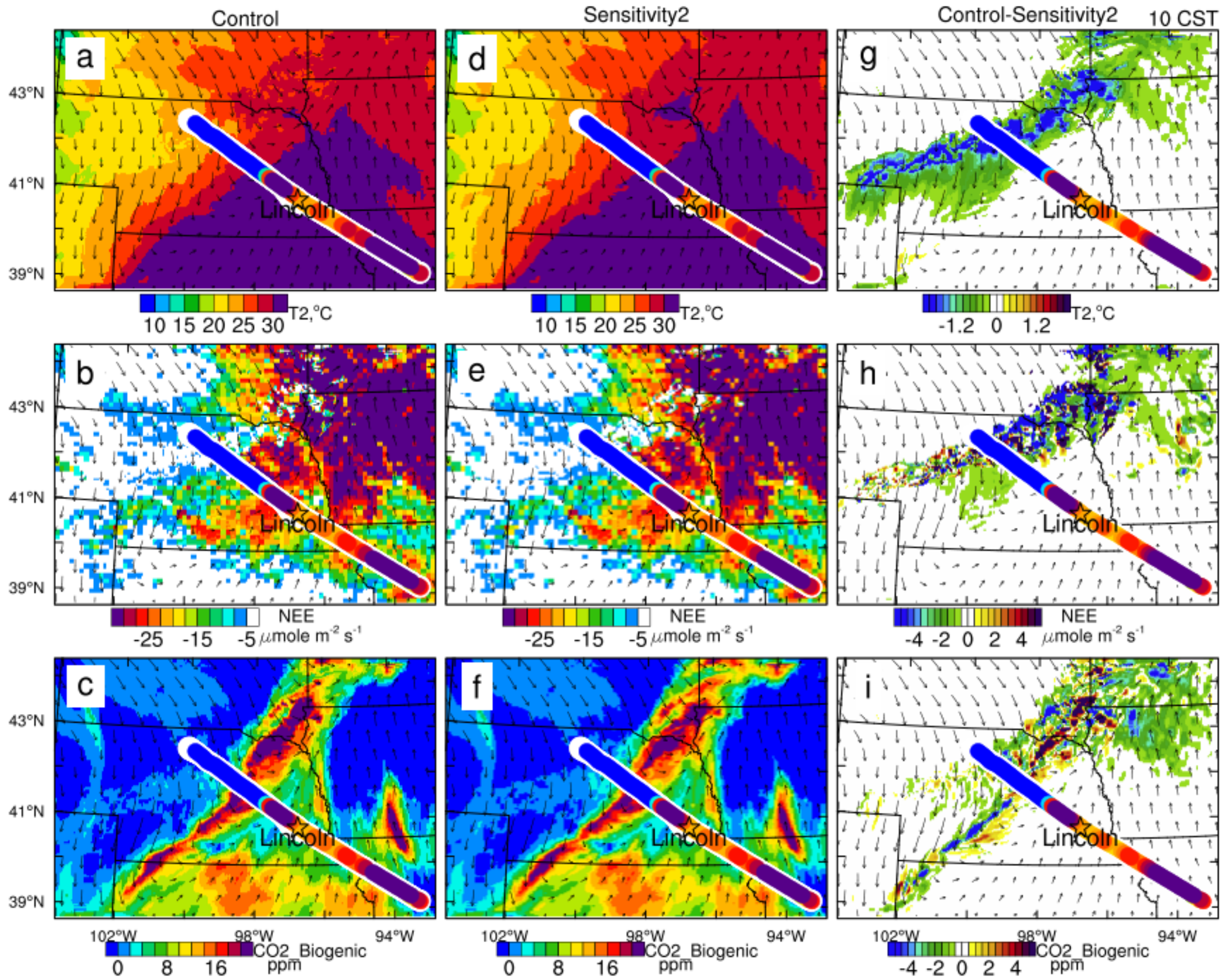

Figure 18. (top to bottom) temperature at 2 m AGL (T2), NEE, and biogenic CO_2 simulated by (left) control and (middle) the clear-sky-surface-energy sensitivity simulation, and (right) their difference at 10 CST. B200 aircraft CO_2 data in the boundary layer at ~12 CST is overlaid.