

# Regional inversion shows promise in capturing extreme-event-driven CO<sub>2</sub> flux anomalies but is limited by atmospheric CO<sub>2</sub> observational coverage

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## Key Points:

- Bottom-up and top-down methods independently capture reduced 2019 US Midwest carbon uptake
- Gaps in atmospheric CO<sub>2</sub> observations drive uncertainties in top-down estimates
- Nested inversion better localizes US Midwest  $\Delta$ NEE relative to coarse global model

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## Abstract

Extreme climate events are becoming more frequent, with poorly understood implications for carbon sequestration by terrestrial ecosystems. A better understanding will critically depend on accurate and precise quantification of ecosystems responses to these events. Taking the 2019 US Midwest floods as a case study, we investigate current capabilities for tracking regional flux anomalies with “top-down” inversion analyses that assimilate atmospheric CO<sub>2</sub> observations. For this analysis, we develop a regionally nested version of the NASA Carbon Monitoring System-Flux (CMS-Flux) that allows high resolution atmospheric transport ( $0.5^\circ \times 0.625^\circ$ ) over a North America domain. Relative to a 2018 baseline, we find US Midwest growing season net carbon uptake is reduced by 11-57 TgC (3–16%) for 2019 (inversion mean estimates across experiments). These estimates are found to be consistent with independent “bottom-up” estimates of carbon uptake based on vegetation remote sensing. We then investigate current limitations in tracking regional carbon emissions and removals by ecosystems using “top-down” methods. In a set of observing system simulation experiments, we show that the ability to recover regional carbon flux anomalies is still limited by observational coverage gaps for both in situ and satellite observations. Future space-based missions that allow for daily observational coverage across North America would largely mitigate these observational gaps, allowing for improved top-down estimates of ecosystem responses to extreme climate events.

## Plain Language Summary

Extreme climate events, such as floods or heatwaves, can have major impacts on the carbon cycle. For example, widespread flooding in the US Midwest during 2019 delayed the planting of crops leading to reduced plant growth and carbon uptake relative to 2018. Here, we test how well this reduction in carbon uptake can be inferred from measurements of atmospheric CO<sub>2</sub>. We find that these data can identify reduced net carbon uptake to the US Midwest during the 2019 floods, but that sparse observational coverage limits our ability to quantify the anomaly in net carbon uptake.

## 1 Introduction

Extreme events, including heat and precipitation extremes, are becoming more frequent (Shenoy et al., 2022; Q. Sun et al., 2021; Kirchmeier-Young & Zhang, 2020; Seneviratne et al., 2021). These events have significant implications for carbon sequestration in terrestrial ecosystems, often causing carbon losses in a single year equal to many years of carbon sequestration (Ciais et al., 2005; Byrne et al., 2021). This is concerning because Nature-based Climate Solutions (NbCSs), which aim to enhance the terrestrial carbon sink through improved land management, have been proposed as an important tool to mitigate CO<sub>2</sub> emissions (Fargione et al., 2018). The increasing frequency of extreme events may disrupt this process, creating a carbon-climate feedback where extreme-event-driven carbon emissions reduce the effectiveness of NbCSs (Zscheischler et al., 2018; Barkhordarian et al., 2021). Consequently, there is an urgent need to quantify the impact of extreme events on carbon uptake by ecosystems for policy programs and other climate applications.

“Top-down” methods offer an approach for estimating biosphere-atmosphere CO<sub>2</sub> fluxes based on observations of atmospheric CO<sub>2</sub>. Typically, Bayesian inverse methods are used to estimate optimal surface fluxes based on constraints from prior information and atmospheric CO<sub>2</sub> observations. Although historically data limited, these techniques are increasingly used to quantify regional carbon cycle responses to extreme events, thanks to expansions of in situ CO<sub>2</sub> measurements and the introduction of space-based retrievals of column-averaged dry-air CO<sub>2</sub> mole fractions ( $X_{\text{CO}_2}$ ) from missions like the Orbiting Carbon Observatory 2 (OCO-2) (Feldman et al., 2023; Byrne et al., 2021). Still, current

capabilities for tracking extreme events are not well understood. This study aims to improve our characterization of these capabilities and identify current limitations.

As a case study, we examine the 2019 US Midwest floods. Intense precipitation during that spring ( $> 2\sigma$  above average) led to widespread flooding across the US Midwest, a region that accounts for 40% of world corn and soybean production (Yin et al., 2020). Inundation delayed crop planting by 2–3 weeks relative to 2018 across the region, with an additional reduction of 6.8 million hectares in the total planted area. These factors led to a 16-day shift in the seasonal cycle of photosynthesis relative to 2018, along with a 15% lower peak value (Yin et al., 2020). In turn, crop yields across the US Midwest were reduced by  $\sim 14\%$ , and a decrease in net carbon uptake of  $\sim 0.1$  PgC was inferred relative to the preceding years (Yin et al., 2020; Balashov et al., 2022). The relatively simple (delayed planting) and well documented carbon cycle perturbation during this event makes it an ideal case study for studying our ability to quantify carbon cycle perturbations using top-down and bottom-up methods.

To perform our analysis, we introduce a regionally nested version of the CMS-Flux inversion system with high-resolution ( $0.5^\circ \times 0.625^\circ$ ) atmospheric transport over North America (see Sec. 2.1). This version offers advantages over the coarse-resolution ( $4^\circ \times 5^\circ$ ) global version of CMS-Flux. It reduces transport errors introduced by the coarsening of reanalysis winds (Stanevich et al., 2020; K. Yu et al., 2018) and better represents assimilated  $\text{CO}_2$  observations, resulting in improved localization of extreme-event-driven  $\text{CO}_2$  flux anomalies (Sec. 3.2.2).

The first objective of this study is to evaluate how well existing atmospheric observing systems can quantify flood-induced reductions in carbon uptake during 2019 relative to 2018. We conduct four inversions that assimilate (1) in situ  $\text{CO}_2$  measurements (IS), (2) OCO-2 land  $X_{\text{CO}_2}$  retrievals (LNLG), (2) both in situ and OCO-2 land data (LNLGIS), or (4) in situ, OCO-2 land and ocean data (LNLGOGIS) (Sec. 2.1). Climatological prior fluxes are employed in each experiment, allowing us to attribute posterior anomalies in carbon uptake between years solely to the assimilation of atmospheric  $\text{CO}_2$  data. We then compare these estimates with an independent ensemble of remote-sensing bottom-up estimates and with crop-yield data to assess their overall consistency (Sec. 3.1).

The second objective of this study is to assess the impact of existing observational coverage gaps and the potential expansion of space-based  $X_{\text{CO}_2}$  measurements on our ability to detect extreme-event-driven anomalies in  $\text{CO}_2$  fluxes. To evaluate the effect of expanded space-based observations, we devise a hypothetical observing system that provides daily  $X_{\text{CO}_2}$  retrievals at 13:00 local time (similar to OCO-2). Subsequently, we conduct observing system simulation experiments (OSSEs) for existing in situ data and OCO-2 data as well as the hypothetical observing system. For each OSSE, we evaluate the effectiveness in capturing extreme-event-driven  $\text{CO}_2$  flux anomalies (Sec. 3.2.1). Our aim is to gain a deeper understanding of how observational coverage impacts our ability to quantify the influence of extreme events on  $\text{CO}_2$  fluxes.

## 2 Methods

Sec. 2.1 introduces the configuration for the nested North America version of the CMS-Flux atmospheric  $\text{CO}_2$  inversion system, including its application for real data experiments (Sec. 2.1.1) and OSSEs (Sec. 2.1.2). Sec. 2.2 describes remote-sensing bottom-up NEE anomaly estimates used in this study. Sec. 2.3 describes the state crop production estimates.

## 2.1 Top-down $\Delta$ NEE estimate

We establish a one-way nested inversion system covering the North America region, spanning from  $40^\circ\text{W}$  to  $167.5^\circ\text{W}$  and  $14^\circ\text{N}$  to  $76^\circ\text{N}$ . Within this domain, model transport is conducted at a spatial resolution of  $0.5^\circ \times 0.625^\circ$  with a five-minute timestep, using archived MERRA-2 reanalysis data. We employ four-dimensional variational data assimilation (4D-Var) to optimize scaling factors on prior land and ocean fluxes. These fluxes are optimized at a coarser spatial and temporal resolution compared to the nested model transport. Spatially, a mask is applied to optimize fluxes over a  $4^\circ \times 5^\circ$  grid, which is truncated at the land-ocean boundary. Temporally, we utilize a six-week inversion window and optimize weekly mean land and ocean scaling factors. The middle four weeks of the inversion window are retained as optimized fluxes, while the first and last weeks are excluded as spin-up and spin-down periods. We conduct a batch of eight six-week inversions offset by four weeks, yielding continuous fluxes from April 8th to November 18th for both 2018 and 2019, resulting in a total of 16 inversion runs.

For each experiment, the nested inversion setup is run three times using different prior fluxes (the BCs and ICs also differ for the real-data experiments, see Sec. 2.1.1). The prior NEE fluxes are derived from the posterior NEE fluxes of the GOSAT+surface+TCCON experiment by Byrne et al. (2020) and differ based on the employed prior NEE (CASA, SiB3, or FLUXCOM). A climatological seasonal cycle is calculated for each prior NEE flux over the period of 2010-2015. Subsequently, the climatological NEE seasonal cycle is partitioned into net primary production (NPP) and heterotrophic respiration (HR) components by subtracting the 2010-2015 mean seasonal cycle from the mean bottom-up NPP estimate (assumed to be 65% of mean GPP estimate here). In the inversions, we impose both the NPP and HR fluxes in the forward simulation, but optimize scaling factors only on the weekly mean HR fluxes. This choice is driven by the improved performance of this configuration during the spring and fall when NEE is close to zero, requiring large scaling factors to adjust the NEE flux. The posterior HR fluxes are not interpreted independently but combined with the prior NPP fluxes to obtain a posterior estimate of NEE for analysis. We generate prior uncertainties on the HR fluxes based on the full range of the three prior NEE fluxes. Prior ocean fluxes are derived similarly from the posterior ocean flux estimates of the GOSAT+surface+TCCON experiment by Byrne et al. (2020), and uncertainties on these estimates reflect the range among the three experiments that employ different NEE priors. The prior fluxes, posterior fluxes, and associated uncertainties are provided as supporting information.

In addition to the ocean, NPP, and HR fluxes, the forward simulations incorporate prescribed fossil fuel emissions, biomass burning emissions, biofuel emissions, and diurnal NEE. Fossil Fuel emissions used here were specifically made for the v10 OCO-2 modelling intercomparison project (MIP) (Byrne et al., 2023; Basu & Nassar, 2021). Biomass burning emissions are derived from the Global Fire Emissions Database version 4 (GFED4.1s) and scaled to incorporate diurnal variations in emissions (van der Werf et al., 2017). Biofuel emissions are obtained from the CASA-GFED4-FUEL dataset. Diurnal variations in NEE are based on the diurnal NEE variations from the CASA and SiB3 models, as described in Byrne et al. (2020). The SiB3 diurnal cycle is employed for the SiB3-based and FLUXCOM-based NEE priors, while the CASA diurnal cycle is prescribed for the CASA-based inversion. All of these fluxes are regridded from their native spatial resolution to  $0.5^\circ \times 0.625^\circ$  (fossil fuel emissions were at  $1.0^\circ \times 1.0^\circ$  degrees, biomass burning emissions were at  $0.25^\circ \times 0.25^\circ$  degrees, and remaining fluxes were at  $4^\circ \times 5^\circ$  as archived by Byrne et al. (2020)).

### 2.1.1 Real data experiment

First, we require atmospheric  $\text{CO}_2$  boundary and initial conditions for the nested model. To generate these conditions, we conduct a global  $4^\circ \times 5^\circ$  4D-Var inversion that

optimizes scaling factors on prior land and ocean fluxes. These global inversions utilize the same configuration as Byrne et al. (2020). The resulting optimized global NEE and ocean fields are then employed in a  $2^\circ \times 2.5^\circ$  global simulation to produce boundary conditions and initial conditions for the nested domain. The global inversions are performed three times, corresponding to each of the three prior NEE estimates. The nested inversion setup is subsequently executed three times using the three different prior fluxes, boundary conditions, and initial conditions based on the three distinct prior flux estimates.

Four sets of experiments are conducted, differing in the assimilated data. The “IS” experiment assimilates in situ  $\text{CO}_2$  measurements from the global network of sites as described below. The “LNLG” experiment assimilates OCO-2 land data, including nadir and glint retrievals. The “LNLGIS” experiment assimilates both in situ and OCO-2 land data. Lastly, the “LNLGOGIS” experiment assimilates in situ, OCO-2 land data, and OCO-2 ocean glint retrievals.

In situ  $\text{CO}_2$  measurements are obtained from version 8.0 of the NOAA GLOBALVIEW plus Obspack dataset (Schuldt et al., 2022). These data are provided on the X2019  $\text{CO}_2$  scale but were back corrected to the X2007  $\text{CO}_2$  scale following Hall et al. (2021). We apply several filters to the in situ data before assimilation. Surface in situ  $\text{CO}_2$  measurements are assimilated at their respective height above the surface, with inclusion criteria that the model surface elevation should differ by less than 500 m from the 15 arc-second ETOPO1 global elevation dataset (NOAA, 2021). Secondly, we only assimilate data with the CT\_assim flag greater than or equal to one, which indicates data that is deemed assimilable for the NOAA CarbonTracker system. Finally, only measurements obtained between 11:00 and 17:00 local time are assimilated (when the atmospheric boundary layer is well mixed). The sites assimilated are: amt, bck, bmw, bra, brw, cba, cby, chl, cps, crv, egb, esp, est, etl, fsd, inu, inx, key, kum, lef, lew, llb, sct, sgp, uta, wbi, wgc, wkt, wsa. The sites with  $\text{CT\_assim} \geq 1$  that are not assimilated are: mbo, mex, mlo, mwo, nwr, omp, uts, wsd. We note that some sites with  $\text{CT\_assim} = 0$  may be assimilable, but more work is needed to characterize their suitability for assimilation. We apply the CT\_MDM “model-data-mismatch” values as uncertainties on assimilated measurements. All aircraft data, including the ACT-America campaign data (Davis et al., 2021, 2018; Wei et al., 2021), are withheld for validation purposes. Monthly maps of data density are shown in Figure S1.

We employ  $X_{\text{CO}_2}$  retrieved using version 10 of NASA’s Atmospheric  $\text{CO}_2$  Observations from Space (ACOS) full-physics retrieval algorithm (O’Dell et al., 2018). Subsequently, OCO-2 “buddy” super-observations are calculated by averaging individual soundings into super-observations at a spatial resolution of  $0.5^\circ \times 0.5^\circ$  within the same orbit, assigning equal weights, following the approach by Liu et al. (2017). Monthly maps illustrating data density are shown in Figure S2.

The global inversions discussed in Sec. 3.2.2 follow an identical set-up as the nested inversions, with the same flux datasets regridded to  $4^\circ \times 5^\circ$  globally.

### 2.1.2 Observing System Simulation Experiments

A series of OSSEs are conducted to explore the impact of observational coverage in quantifying carbon cycle perturbations resulting from extreme events. These OSSEs cover the same two year period as the real data inversions. Four OSSE experiments are carried out: IS, LNLG, LNLGOGIS, and one for a new hypothetical space-based observing system that provides daily  $X_{\text{CO}_2}$  retrievals at 13:00 (1 pm). This hypothetical system, referred to as the ideal LEO mission, could comprise a dense constellation of low Earth orbit (LEO) sensors. The OSSEs are carried out following the same setup as the real data experiments, while the true atmospheric  $\text{CO}_2$  boundary and initial conditions are implemented for the nested inversion.

For the ideal LEO mission, pseudo-observations are generated as follows: 1 pm observations within each land  $0.5^\circ \times 0.625^\circ$  grid cell are filtered to exclude instances of low-light conditions, cloudy conditions, and when the surface is covered by snow or ice. Fractional snow cover and cloud cover data are obtained from the MERRA-2 reanalysis dataset (Gelaro et al., 2017). Measurements are excluded for grid cells with a fractional area of land snow cover (FRSNO) greater than 75% and total cloud area fraction (ISCCPCLD-FRC) greater than 75% from the International Satellite Cloud Climatology Project (ISCCP). Additionally, observations with an atmospheric path exceeding six air-masses are removed. We allow one super-obs within each gridcell per day. The uncertainty on the super-obs is defined to be 0.7 ppm, roughly matching OCO-2. Monthly maps of data density for the ideal LEO mission are shown in Fig. S3.

True NEE fluxes for the OSSEs are generated by combining a climatological NEE seasonal cycle with anomalies from the bottom-up datasets. Climatological true NEE fluxes are obtained from the CASA-GFED3 model, which undergoes downscaling from monthly to three-hourly fluxes. These fluxes align with those described in Appendix 3 of Byrne et al. (2020). Interannual variations in the true fluxes are introduced by incorporating NEE anomalies taken to be 65% of the mean bottom-up GPP anomalies across the five datasets (see Sec. 2.2). Pseudo-observations are then generated by conducting a forward simulation using the nested model.

## 2.2 Remote-sensing bottom-up $\Delta$ GPP and $\Delta$ NEE estimates

We generate an ensemble of five bottom-up  $\Delta$ GPP estimates by combining a number of remote-sensing-based GPP datasets. Four of these are obtained from existing datasets: 8 day FLUXCOM remote-sensing-based (RS) GPP (Jung et al., 2020), FluxSat Version 2 (Joiner & Yoshida, 2020), GOSIF GPP (Li & Xiao, 2019), and the NIR<sub>V</sub>-based GPP estimates of L. He et al. (2022). All of these data are regridded from their native resolution to weekly temporal resolution and  $0.5^\circ \times 0.625^\circ$  spatial resolution.

In addition, we estimate GPP directly from TROPOMI SIF data. This followed the same approach as Yin et al. (2020). Two GPP estimates are then calculated using land-cover-dependent SIF-to-GPP scaling factors from Li et al. (2018) and Y. Sun et al. (2017), which were adjusted by a factor of 0.64 to account for difference retrieval wavelengths between OCO-2 and TROPOMI (740 nm vs 757 nm). These factors were then applied to gridded SIF data (0.08333° spatial and 8 day temporal resolution), while accounting for the fractional vegetation cover within each gridcell. The GPP estimates were then regridded to  $0.5^\circ \times 0.625^\circ$  spatial resolution. Any data gaps within the growing season are then filled by linear interpolation over time, while GPP is assumed to be zero for data gaps outside the growing season. Finally the two GPP estimates are averaged.

From these GPP datasets, we estimate an anomaly in NEE between 2018 and 2019 by assuming the NEE anomaly is equal to the NPP anomaly, which is itself related to the GPP anomaly by:

$$\Delta\text{NEE} = -\Delta\text{NPP} = -0.60 \times \Delta\text{GPP} \quad (1)$$

The factor of 0.60 is an estimate of the carbon use efficiency (CUE), and is a relatively high estimate (Manzoni et al., 2018; Y. He et al., 2018), though may be representative of corn (S. Yu et al., 2023; Campioli et al., 2015). We assume an error of  $\pm 0.1$  in CUE, and perform error analysis using factors of 0.5 and 0.7. The conversion of  $\Delta$ NPP to  $\Delta$ NEE assumes that  $\Delta$ HR is negligible. This is likely a poor assumption, but a limitation of remote-sensing estimates that are insensitive to HR variations. Previously, Yin et al. (2020) showed that bottom-up  $\Delta$ NEE estimated assuming negligible  $\Delta$ HR could reasonably reproduce observed atmospheric CO<sub>2</sub> enhancements during the 2019 US Midwest floods, providing some evidence that  $\Delta$ HR variations have a secondary impact.



### 2.3 State crop yields and NPP

Crop yields, which represents the amount of crop biomass removed from the field during harvest events, have been estimated using county-level crop yield data from the US Department of Agriculture (USDA) - National Agricultural Statistics Service (NASS) (USDA-NASS, 2020). The carbon content of crop yields was derived from the relationship:

$$Y_C = Y_{\text{NASS}} \times \text{DM} \times C_f, \quad (2)$$

where  $Y_C$  is the crop yield, in units of carbon,  $Y_{\text{NASS}}$  is the annual county-level crop yield data from USDA-NASS, DM is the dry matter content for each crop, and  $C_f$  is carbon content crop factor. Crop NPP ( $\text{NPP}_{\text{crop}}$ ), representing the net carbon uptake by crops, was derived from the crop yield estimates using the following equation:

$$\text{NPP}_{\text{crop}} = Y_{\text{NASS}} \times \frac{1}{\text{HI}} \times (1 + \text{RRS}) \times \text{DM} \times C_f, \quad (3)$$

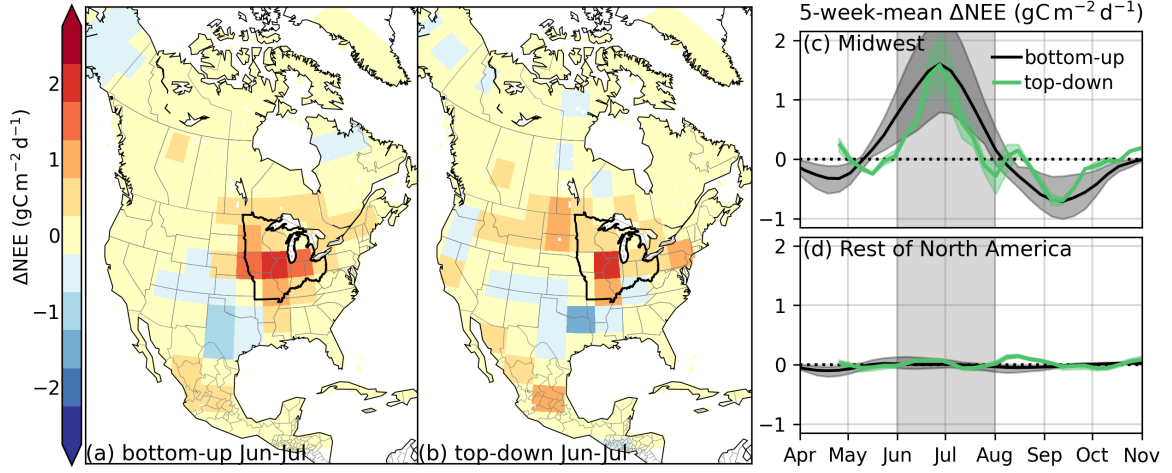
where HI is the harvest index for each crop, i.e., the proportion of harvested material (e.g., grains) in relation to total crop aboveground biomass; and RRS is the root:shoot ratio for each crop. We used crop-specific factors for dry matter, root:shoot ratios, harvest indices, and carbon content following the methods in West et al. (2010, 2011) and Ogle et al. (2015). Crop yields and NPP were estimated for over 20 crops, which together represented >99% of total US crop production (USDA-NASS, 2020). Uncertainty in estimates were propagated through a Monte Carlo approach with 10,000 replicates and probability distribution functions for all input data and factors. The results are based on the mean and 95% confidence intervals from the final distribution of simulated values. We note that NASS only included uncertainty in crop yield data for 2020 so we assumed a similar level of uncertainty in crop yields for the other years.

## 3 Results

### 3.1 Flood-induced NEE anomalies

Figure 1a–b illustrates the difference in June–July NEE between 2019 and 2018 ( $\Delta\text{NEE} = \text{NEE}_{2019} - \text{NEE}_{2018}$ ) for both the remote-sensing bottom-up (ensemble mean) and top-down (LNLGOGIS) estimates. The analyses reveal a significant decrease in  $\text{CO}_2$  uptake (positive  $\Delta\text{NEE}$ ) specifically in the US Midwest region. This pronounced positive  $\Delta\text{NEE}$  signal in the US Midwest stands out compared to the rest of the continent. Figure 1c presents the 5 week running mean time series of  $\Delta\text{NEE}$  over the US Midwest. Both the top-down and bottom-up estimates depict a positive  $\Delta\text{NEE}$  signal throughout Jun–Jul, with the anomaly peaking towards the end of June. However, during Aug–Sep, the top-down and bottom-up estimates suggest a negative  $\Delta\text{NEE}$  in the US Midwest. Across the rest of the continent (Figure 1d), anomalies are weaker. The top-down estimate suggests a positive anomaly outside the US Midwest during August, while the bottom-up estimate suggests no significant anomalies. The supplementary materials display the maps and timeseries for the other top-down experiments (Fig. S4) and individual bottom-up datasets (Fig. S5).

Figure 2 shows US Midwest  $\Delta\text{NEE}$  for each of the top-down and bottom-up estimates. In addition, an estimate of the anomaly in net primary production for crops ( $\Delta\text{NPP}_{\text{crop}}$ ) derived from crop yield data is shown. All estimates suggest positive  $\Delta\text{NEE}$  over the study period (-6–85 TgC for top-down, 15–78 TgC for bottom-up, and 36–65 TgC for yield-based estimates). We find that June–July  $\Delta\text{NEE}$  drives the annual anomaly with uptake reduced by 24–76 TgC in top-down estimates and 38–131 TgC in bottom-up estimates. The bottom-up estimates suggest this is moderated when integrating across the growing season due to greater carbon uptake during Aug–Sep (-56 TgC to -15 TgC), while the top-down estimates are less consistent during Aug–Sep, ranging from -37 TgC to 34 TgC. Figure S6 demonstrates that the bottom-up and top-down  $\Delta\text{NEE}$  generally show similar June–July  $\Delta\text{NEE}$  across the CONUS Climate Assessment Regions. In particular, we



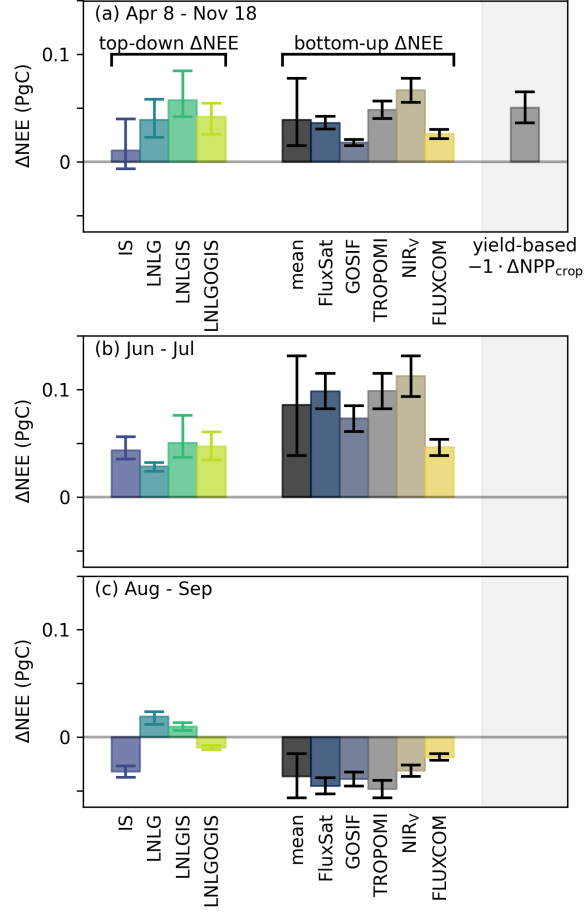
**Figure 1.** (a) Bottom-up and (b) top-down (LNLGOGIS) spatial patterns of June–July mean  $\Delta\text{NEE}$  ( $\text{NEE}_{2019} - \text{NEE}_{2018}$ ) at  $4^\circ \times 5^\circ$  spatial resolution. (c) US Midwest and (d) rest of North America 5-week-mean  $\Delta\text{NEE}$ . The US Midwest is defined as the area within Illinois, Indiana, Iowa, Michigan, Minnesota, Missouri, Ohio, and Wisconsin and is indicated by the black outline in panels (a) and (b). The shading shows the range around the mean estimate for the inversions using three different priors and for the five bottom-up GPP datasets.

find that all estimates obtain negative  $\Delta\text{NEE}$  across the Southern Great Plains (-22 to -46 TgC), resulting from the 2018 drought (Turner et al., 2021).

These findings suggest that both in situ and OCO-2 data provide adequate observational coverage to detect the June–July  $\Delta\text{NEE}$  signal resulting from the 2019 US Midwest floods. However, some differences are also evident. The experiments disagree in the sign of Aug–Sep  $\Delta\text{NEE}$ . The IS experiment shows negative Aug–Sep  $\Delta\text{NEE}$  that largely compensates for the positive June–July  $\Delta\text{NEE}$ . Conversely, the LNLG experiment gives positive Aug–Sep  $\Delta\text{NEE}$  but the smallest June–July  $\Delta\text{NEE}$ . There are some spatial differences as well, for example, the IS experiment suggests larger positive  $\Delta\text{NEE}$  in western Canada and negative  $\Delta\text{NEE}$  in the southeast during Jun–Jul than the other experiments (Fig. S4). The LNLGIS and LNLGOGIS experiments yield quite similar results. The relative accuracy of these different estimates is challenging to evaluate, as a number of different drivers could contribute to differences but all experiments exhibit good agreement with independent aircraft  $\text{CO}_2$  measurements during 2018 and 2019 (Text S1, Fig. S7–S12). The disparities between experiments may arise from differences in observational coverage and this hypothesis is examined in Sec. 3.2.1.

The bottom-up estimates show some notable differences in the magnitude of  $\Delta\text{NEE}$  over the US Midwest and the spatial structure of  $\Delta\text{NEE}$  outside the US Midwest (Fig. S5). FLUXCOM consistently displays the weakest  $\Delta\text{NEE}$  signal, and has been previously shown to underestimate interannual variations in NEE and GPP (Jung et al., 2020). Outside the US Midwest, the  $\text{NIR}_V$ -based estimate shows negative values across the western half of North America, which are not observed in any other estimates, while the TROPOMI-based estimate indicates positive  $\Delta\text{NEE}$  across a large portion of eastern Canada. Consequently, the net June–July  $\Delta\text{NEE}$  signal outside the US Midwest varies across datasets, ranging from -218 TgC to 187 TgC.





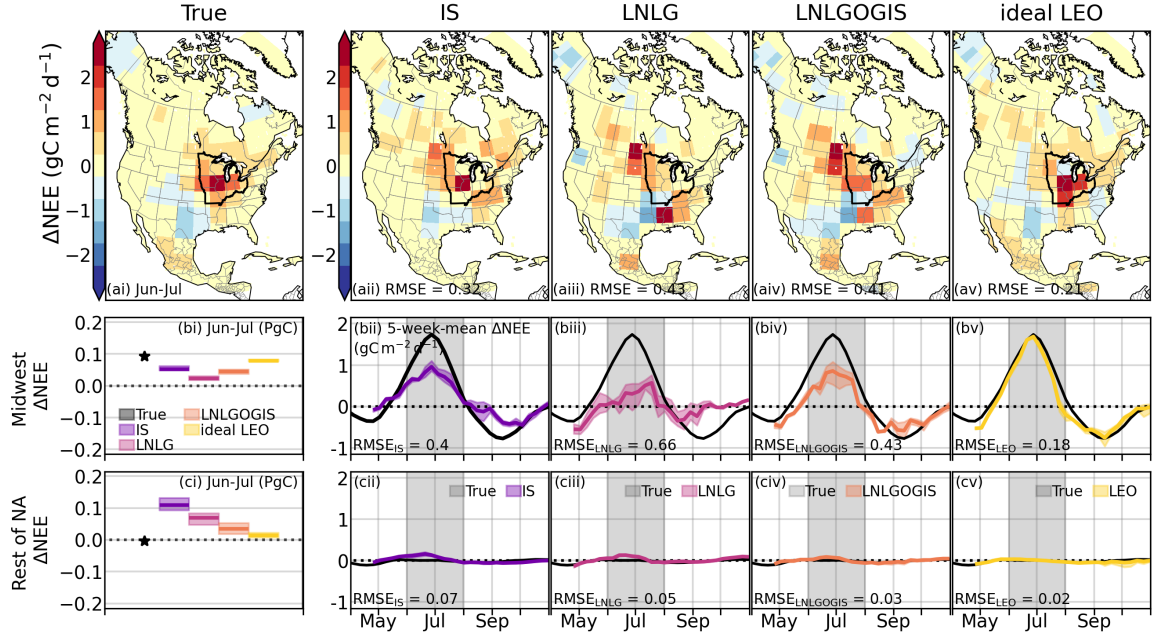
**Figure 2.** Top-down  $\Delta\text{NEE}$ , bottom-up  $\Delta\text{NEE}$ , and yield-based  $\Delta\text{NPP}$  for crops ( $\Delta\text{NPP}_{\text{crop}}$ ) over the US Midwest.  $\Delta\text{NEE}$  is calculated for (a) the entire inversion period (April 8th – Nov 18th), (b) June-July and (c) Aug-Sep. The top-down estimates show the mean and range obtained using three different priors. Uncertainty bars for the top-down estimates show the range using three priors, while the uncertainties on the bottom-up show the range of using carbon use efficiencies of 0.5–0.7.

## 3.2 Sensitivity experiments

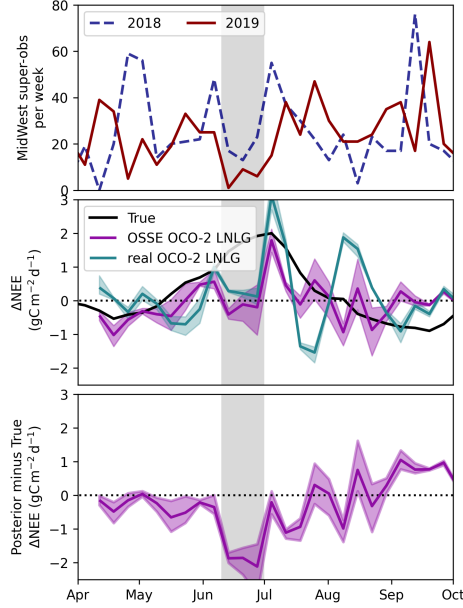
### 3.2.1 Impact of observational coverage

Although both the in situ network and OCO-2 were able to identify a positive US Midwest  $\Delta\text{NEE}$  signal, we found substantial differences between the top-down experiments. Here we perform OSSEs to investigate whether gaps in observational coverage could explain these differences. Further, we test whether increased observational coverage (in an ideal LEO constellation) would substantially improve top-down estimates of extreme-event-driven carbon cycle perturbations.

Figure 3 shows the true and posterior  $\Delta\text{NEE}$  for the OSSEs. All OSSEs recover positive  $\Delta\text{NEE}$  to the US Midwest, consistent with the real data experiments. However, June–July US Midwest  $\Delta\text{NEE}$  is underestimated by 43% for IS, 75% for LNLG, 48% for LNLGOGIS and 15% for the ideal LEO constellation. In addition, the inversions tend to introduce a positive June–July  $\Delta\text{NEE}$  outside the US Midwest that is not present in the truth. Over June–July, the true continental-scale  $\Delta\text{NEE}$  is 89 TgC, while the mean inversion estimates are 163 TgC (error of +74 TgC) for IS, 93 TgC (error of +4 TgC) for LNLG, 68 TgC (error of -21 TgC) for LNLGOGIS, and 93 TgC (error of +4 TgC) for ideal LEO. A similar large continental-scale positive June–July  $\Delta\text{NEE}$  was found for the real data IS experiment (Fig. S4ci). One possible explanation is that the limited spatial coverage of the in situ (Fig. S1) data may limit the ability to capture aggregate continental-scale budgets using a one-way nested system.



**Figure 3.**  $\Delta\text{NEE}$  estimates for the OSSEs. Panel (ai) shows the true June–July  $\Delta\text{NEE}$  maps, while panels (aii)–(av) show the OSSE posterior June–July  $\Delta\text{NEE}$  maps and RMSE across grid-cells ( $\text{gC m}^{-2} \text{d}^{-1}$ ). The net US Midwest Jun–Jul  $\Delta\text{NEE}$  (PgC) is shown for each OSSE in panel (bi), and the timeseries of 5-week-mean  $\Delta\text{NEE}$  is shown for each experiment in panels (bii)–(bv), with RMSE across weeks ( $\text{gC m}^{-2} \text{d}^{-1}$ ). The same quantities are shown for the rest of North America in panels (ci)–(cv).



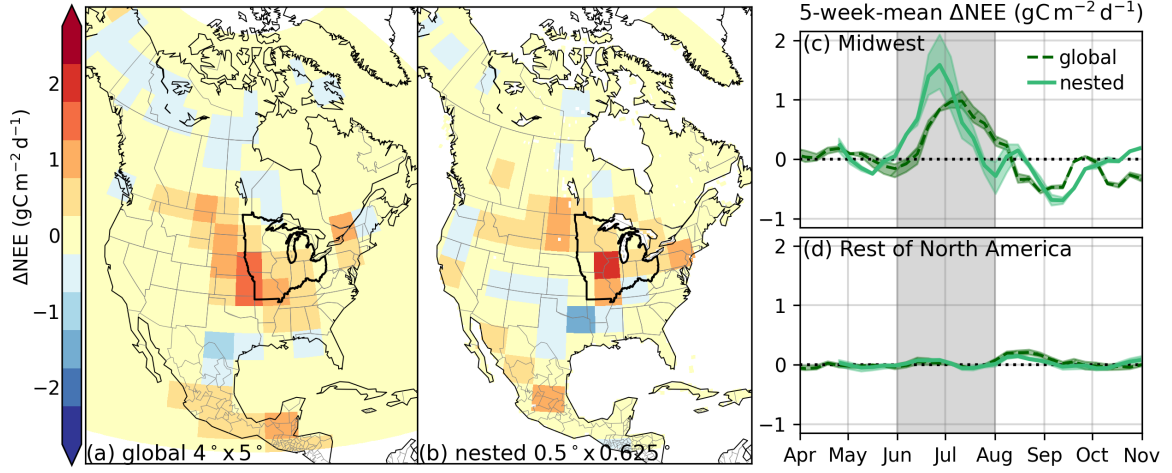
**Figure 4.** Weekly timeseries of (top) number of OCO-2 super-obs in the US Midwest for 2018 and 2019. (middle) Weekly  $\Delta\text{NEE}$  in the US Midwest for the truth, OCO-2 OSSE and real OCO-2 LNLG experiment. (bottom) Difference between posterior and true  $\Delta\text{NEE}$  for the OCO-2 OSSE. The shading shows the range around the mean estimate for the inversions using three different priors.

Overall, the LNLG OSSE shows the worst performance at isolating the US Midwest  $\Delta\text{NEE}$ . We suggest that this could be related to interannual variations in the observational coverage. Figure 4a shows that the number of LNLG weekly samplings over the US Midwest can be quite variable from year to year. In particular, there are only 16 super-obs in the US Midwest during the three week period of June 11, 2019 to July 2 2019. This coincides with near zero  $\Delta\text{NEE}$  for both the real data LNLG inversion and OSSE (Fig. 4b), and the period with the largest error in  $\Delta\text{NEE}$  for the OSSE (Fig. 4c). These results suggest that data gaps in OCO-2, particularly differences in observational coverage between years, limit our ability to estimate inter-annual variations in NEE at high spatio-temporal resolution.

The increased sampling from combining the datasets (LNLGOGIS) appears to moderately improve performance, particularly in isolating June–July  $\Delta\text{NEE}$  to the US Midwest (relative to LNLG) and better capturing the continental-scale  $\Delta\text{NEE}$  (relative to IS). However, the ideal LEO constellation results in much improved performance in both space and time. The ideal LEO constellation reduces June–July RMSE across  $4^\circ \times 5^\circ$  regions by 34–51% and the 5-week-mean  $\Delta\text{NEE}$  US Midwest RMSE by 55–73%. This comparison suggests that top-down estimates of extreme-event-driven perturbations to carbon uptake remain observationally-limited and that expanded space-based observing systems will improve these estimates.

### 3.2.2 Comparison between nested and global inversions

The nested CMS-Flux inversion system in this study offers both advantages and disadvantages compared to a global CMS-Flux inversion system. One major advantage is the ability to run transport at a higher resolution ( $0.5^\circ \times 0.625^\circ$ ) compared to the global



**Figure 5.** Comparison of the global 4° × 5° and nested inversion results. Maps of June–July  $\Delta\text{NEE}$  from the LNLGOGIS experiment are shown for (a) the global 4° × 5° inversion and (b) the nested inversion. Weekly  $\Delta\text{NEE}$  in the US Midwest after applying a 5-week running mean are also shown for (c) the US Midwest and (d) rest of North America.

system (4° × 5°). This higher resolution enables tracer transport to be closer to the parent model, as spatial averaging of meteorological fields can average out eddy transport, particularly affecting vertical motions (Stanevich et al., 2020). Additionally, a higher resolution model grid reduces representativeness errors, allowing better representation of fine-scale features that influence observations, such as topography. The primary disadvantage of the one-way nested system used in this study is the assumption of perfect boundary conditions and the inability to assimilate atmospheric CO<sub>2</sub> observations outside the nested domain. In a global inversion, fluxes over North America would impact measurements downwind, providing a powerful constraint on large-scale fluxes, including the net North American flux (Liu et al., 2015). A bias in flux at the continental scale would affect CO<sub>2</sub> fields across the entire Northern Hemisphere. Since the nested inversion lacks this constraint, significant errors in continental-scale fluxes may go undetected. Furthermore, biases in the imposed boundary CO<sub>2</sub> fields can propagate into optimized fluxes.

In order to assess the performance of the one-way nested inversion, we compare the obtained  $\Delta\text{NEE}$  with the global version of CMS-Flux using the same inversion configuration, whenever possible. Figure 5 presents the results for both the global and nested versions of CMS-Flux. It is observed that the nested version of CMS-Flux effectively isolates  $\Delta\text{NEE}$  to the US Midwest region during June–July. In contrast, the global model exhibits spatially broader positive  $\Delta\text{NEE}$  across the US Midwest and Great Plains, resulting in a significantly reduced  $\Delta\text{NEE}$  estimate for the US Midwest during June–July. The spatial pattern of  $\Delta\text{NEE}$  for the nested model aligns more closely with the bottom-up estimate, suggesting that this system better captures the overall event. This indicates that, considering the observational coverage provided by LNLGOGIS, the benefits of reduced transport and representativeness errors in the nested model outweigh the detrimental impact of a limited domain.

We note that achieving good performance with nested version of CMS-Flux was challenging, and required a number of trial-and-error inversions. This included varying the size of the state vector spatially (0.5° × 0.625° versus 4° × 5° grid) and temporally (weekly, bi-weekly, monthly intervals). It also involved adjusting the prior constraints (optimizing HR rather than NEE, adjusting prior uncertainties). We suggest that these

challenges are due to greater regularization requirements for the nested model in comparison to the global model. The sensitivities of observations to surface fluxes are limited to 1–2 weeks by the one-way nesting, such that large-scale constraints are imposed by the boundary conditions (Feng, Lauvaux, Davis, et al., 2019; Feng, Lauvaux, Keller, et al., 2019). Thus, the flux signal in the domain is generally much smaller than for the global model, where downwind observations provide important information for upwind continental-scale regions (Liu et al., 2015). We suggest that imposing an error correlation length between state-vector elements may be an effective approach for regularization in a nested inversion context (see Sec. 4.1), however, this is beyond the scope of our current study.

## 4 Discussion and Conclusions

Both top-down and bottom-up approaches capture a flood-induced reduction in net carbon uptake during the 2019 US Midwest floods. The top-down approach gave mean estimates of 11 TgC (IS), 39 TgC (LNLG), 57 TgC (LNLGIS), 42 TgC (LNLGOGIS) for US Midwest growing season  $\Delta\text{NEE}$ . Meanwhile, the bottom-up datasets gave a mean estimate of 39 TgC (range: 15–78 TgC). These magnitudes are significant compared to anthropogenic emissions, amounting to as much as 28% of the US Midwest’s annual fossil fuel emissions (300 TgC yr<sup>−1</sup> for 2019, U.S. Energy Information Administration (2023)). In addition, this anomaly is comparable to the year-to-year variations in fossil fuel emissions (SD: 25 TgC yr<sup>−1</sup>), even including the reduction of regional emissions by 36 TgC yr<sup>−1</sup> due to COVID-19 lockdowns in 2020.

In the context of more frequent heat and precipitation extremes (Seneviratne et al., 2021), accurate estimates of the carbon cycle responses will be critical for monitoring carbon budgets and evaluating carbon-climate feedbacks. The results of this study show that both top-down and bottom-up approaches demonstrate skill in capturing  $\Delta\text{NEE}$  resulting from the 2019 Midwest floods, however a number of deficiencies were also identified. In the following sub-sections, we highlight current challenges and opportunities in quantifying carbon cycle extremes.

### 4.1 Top-down

Observational gaps in atmospheric CO<sub>2</sub> observations are identified as a key limitation in applying top-down methods to quantify extreme-event-driven  $\Delta\text{NEE}$ , consistent with recent studies of the European carbon budget (W. He et al., 2023; Munassar et al., 2022; Monteil et al., 2020; Thompson et al., 2020). Through a series of OSSE experiments, it was demonstrated that gaps in both the in situ network and OCO-2 sampling impact the accuracy of  $\Delta\text{NEE}$  estimates. While assimilating these two datasets concurrently partially mitigates the issue, fully resolving the problem requires expanded observations. Coverage similar to the ideal LEO observing system could be developed by combining multiple individual satellites, and motivates future studies that assimilate X<sub>CO<sub>2</sub></sub> retrievals from multiple space-based observing systems concurrently (e.g., GOSAT, OCO-2, and OCO-3). In addition, efforts should be made to ensure consistency in X<sub>CO<sub>2</sub></sub> retrievals between existing and planned missions (e.g., CO2M, GOSAT-GW). Expanding the in situ network would also likely enhance the ability to capture regional flux anomalies more effectively, however, this was not specifically explored.

Although current observing gaps are found to be a major limitation, there may be approaches to better regularize the inverse problem and reduce the impact of these gaps. In particular, applying off-diagonal co-variances in the prior error covariance matrix could be employed to adjust fluxes where observations are missing (Chen et al., 2023). Applying spatial co-variances will likely be especially important for in situ inversions, while applying temporal co-variances may be most useful for OCO-2 X<sub>CO<sub>2</sub></sub> inversions. Of course, such an approach will only improve flux estimates if spatial and temporal co-variances

are truly present, such that this approach will be limited by a correlation length scale. In addition, imposing realistic prior IAV could also be a fruitful approach, as has been done in previous studies evaluating the 2019 US Midwest floods (Yin et al., 2020; Balashov et al., 2022). However, high-confidence is needed in imposed prior IAV, as inaccurate prior IAV can significantly degrade posterior IAV estimates (Byrne et al., 2019). Text S2 and Figs. S13-15 show that imposing bottom-up IAV in the prior results in larger posterior  $\Delta$ NEE anomalies during the Midwest Floods for all experiments. This is consistent with the  $\Delta$ NEE anomalies being underestimated when using climatological priors, as was found in the OSSEs.

Finally, this study investigated the utility of a one-way nested version of CMS-Flux with  $0.5^\circ \times 0.625^\circ$  spatial resolution relative to the global model at  $4^\circ \times 5^\circ$  degree spatial resolution. We note that developing a nested inversion system involved considerable effort in tuning the state vector structure, assimilation window, and prior constraints. Nevertheless, we found that the nested model better allocated flood-induced  $\Delta$ NEE to the US Midwest, suggesting that the improved model transport and observation representation of the nested model improved the overall performance relative to the global model, consistent with several recent studies (Monteil et al., 2020; Hu et al., 2019). However, the nested model has some disadvantages, especially the inability to assimilate downwind observations outside the model domain that may limit the utility of the nested model in other applications. Transport uncertainty and boundary condition errors may lead to significant challenges for nested inversions (Munassar et al., 2023; Kim et al., 2021; Chen et al., 2019; Lauvaux et al., 2012), but were not obvious in our analyses. We note that high-resolution models will be needed to take advantage of upcoming wide-swath sampling missions, such as CO2M ( $\sim 250$  km swath) or GOSAT-GW ( $\sim 400$  km swath).

## 4.2 Bottom-up

Remote-sensing-based bottom-up estimates of  $\Delta$ NEE provided a consistent picture of reduced net uptake during the 2019 Midwest floods but differed significantly in magnitude. The primary source of this variability stems from translating space-based reflectance or SIF observations to GPP, leading to a range in  $\Delta$ GPP between datasets of 120% of the mean. Indeed, estimating the magnitude of GPP from remote sensing datasets is challenging due to satellite signals that could be influenced by factors such as cloud coverage and soil background, in addition to calibration that is predominantly relying on benchmarks provided by eddy covariance sites. We encourage research into approaches that can reduce uncertainties on large-scale GPP magnitudes, possibly through top-down constraints from Carbonyl Sulphide.

Additional uncertainties were introduced in estimating  $\Delta$ NEE from  $\Delta$ GPP. Due to the inherent limitations of remote sensing, which can track GPP but not the total ecosystem respiration (the sum of HR and AR), certain assumptions must be made. First, to estimate AR, we assumed that  $\Delta$ GPP and  $\Delta$ NPP can be related through a constant carbon use efficiency (CUE) parameter that varies across vegetation type, age, and management practices (Campioli et al., 2015; DeLucia et al., 2007; Manzoni et al., 2018; Y. He et al., 2018; S. Yu et al., 2023). In our analysis, we adopted a mean value of 0.60 with an uncertainty of range 20% (0.5–0.7), which encompasses most literature estimates. Second, we assumed that the influence of  $\Delta$ HR on the  $\Delta$ NEE was negligible. The secondary impact of  $\Delta$ HR is supported by Yin et al. (2020), who were able to reasonably reproduce observed atmospheric CO<sub>2</sub> enhancements during the 2019 US Midwest floods while neglecting  $\Delta$ HR variations. Still, it is important to note that HR is sensitive to variations in temperature and moisture. Terrestrial biosphere models could serve as potential tools for estimating  $\Delta$ HR (e.g., Balashov et al. (2022)) as remote sensing does not adequately capture variations in HR, which is significantly influenced by the availability of labile carbon. However, the accuracy of these model-driven estimates remains challenging to verify.



## 5 Open Research

Once accepted for publication, the prior and posterior fluxes, TROPOMI-based GPP, and NIR<sub>V</sub>-based GPP will be archived with a DOI. During the review processes the data are available by contacting Brendan Byrne. The atmospheric CO<sub>2</sub> inversion analyses performed in this study used the CMS-Flux model, which is based on the GEOS-Chem Adjoint model that can be accessed from the GEOS-Chem Wiki (<https://wiki.seas.harvard.edu/geos-chem>). OCO-2 X<sub>CO<sub>2</sub></sub> Lite files can be downloaded from the GES DISC (<https://disc.gsfc.nasa.gov>). In Situ CO<sub>2</sub> measurements (Schuldt et al., 2022) can be downloaded from <https://gml.noaa.gov/ccgg/obspack/>. GFED biomass burning emissions (van der Werf et al., 2017) were downloaded from <https://globalfiredata.org/>. Fossil fuel emissions (Basu & Nassar, 2021) were downloaded from <https://doi.org/10.5281/zenodo.4776925>. MERRA-2 reanalysis data (Gelaro et al., 2017) was downloaded from <https://disc.gsfc.nasa.gov>. TROPOMI SIF data are accessed online at <https://data.caltech.edu/records/1347> (DOI: 10.22002/D1.1347). FluxSat Version 2 (Joiner & Yoshida, 2021) were downloaded from the ORNL DAAC (<https://daac.ornl.gov>). GOSIF GPP (Li & Xiao, 2019) were downloaded from <http://data.globalecology.unh.edu/>. FLUXCOM GPP (Jung et al., 2020) was downloaded from the data portal of the Max Planck Institute for Biogeochemistry (<https://www.bgc-jena.mpg.de/geodb/projects/Home.php>).

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