Improved constraints on northern extratropical CO2 fluxes obtained by combining surface-based and space-based atmospheric CO2 measurements

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Abstract

Top-down estimates of CO2 fluxes are typically constrained by either surface-based or space-based CO2 observations. Both of these measurement types have spatial and temporal gaps in observational coverage that can lead to biases in inferred fluxes. Assimilating both surface-based and space-based measurements concurrently in a flux inversion framework improves observational coverage and reduces sampling biases. This study examines the consistency of flux constraints provided by these different observations and the potential to combine them by performing a series of six-year (2010–2015) CO2 flux inversions. Flux inversions are performed assimilating surface-based measurements from the in situ and flask network, measurements from the Total Carbon Column Observing Network (TCCON), and space-based measurements from the Greenhouse Gases Observing Satellite (GOSAT), or all three datasets combined. Combining the datasets results in more precise flux estimates for sub-continental regions relative to any of the datasets alone. Combining the datasets also improves the accuracy of the posterior fluxes, based on reduced root-mean-square differences between posterior-flux-simulated CO2 and aircraft-based CO2 over midlatitude regions (0.35–0.50 ppm) in comparison to GOSAT (0.39–0.57 ppm), TCCON (0.52–0.63 ppm), or in situ and flask measurements (0.45–0.53 ppm) alone. These results suggest that surface-based and GOSAT measurements give
complementary constraints on CO2 fluxes in the northern extratropics and can be combined in flux inversions to improve observational coverage. This stands in contrast with many earlier attempts to combine these datasets and suggests that improvements in the NASA Atmospheric CO2 Observations from Space (ACOS) retrieval algorithm have significantly improved the consistency of space-based and surface-based flux constraints.
Improved constraints on northern extratropical CO₂ fluxes obtained by combining surface-based and space-based atmospheric CO₂ measurements

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Key Points:

• Consistent flux constraints provided by surface in situ and flask, TCCON, and GOSAT measurements of atmospheric CO₂.
• Combining data sets improves agreement between modeled and measured aircraft-based CO₂ measurements.
• Improvements in NASA ACOS retrieval explain improved consistency of space-based and surface-based CO₂.

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Abstract

Top-down estimates of CO₂ fluxes are typically constrained by either surface-based or space-based CO₂ observations. Both of these measurement types have spatial and temporal gaps in observational coverage that can lead to biases in inferred fluxes. Assimilating both surface-based and space-based measurements concurrently in a flux inversion framework improves observational coverage and reduces sampling biases. This study examines the consistency of flux constraints provided by these different observations and the potential to combine them by performing a series of six-year (2010–2015) CO₂ flux inversions. Flux inversions are performed assimilating surface-based measurements from the in situ and flask network, measurements from the Total Carbon Column Observing Network (TCCON), and space-based measurements from the Greenhouse Gases Observing Satellite (GOSAT), or all three datasets combined. Combining the datasets results in more precise flux estimates for sub-continental regions relative to any of the datasets alone. Combining the datasets also improves the accuracy of the posterior fluxes, based on reduced root-mean-square differences between posterior-flux-simulated CO₂ and aircraft-based CO₂ over midlatitude regions (0.35–0.50 ppm) in comparison to GOSAT (0.39–0.57 ppm), TCCON (0.52–0.63 ppm), or in situ and flask measurements (0.45–0.53 ppm) alone. These results suggest that surface-based and GOSAT measurements give complementary constraints on CO₂ fluxes in the northern extratropics and can be combined in flux inversions to improve observational coverage. This stands in contrast with many earlier attempts to combine these datasets and suggests that improvements in the NASA Atmospheric CO₂ Observations from Space (ACOS) retrieval algorithm have significantly improved the consistency of space-based and surface-based flux constraints.

1 Introduction

Observations of atmospheric CO₂ provide a constraint on the net surface–atmosphere CO₂ flux, and are critical for monitoring carbon flux changes. This has motivated observational programs that measure atmospheric CO₂, including a global network of surface-based in situ and flask monitoring sites, the Total Carbon Column Observing Network (TCCON) of ground-based spectrometers (Wunch et al., 2011) and several satellite missions (Crisp et al., 2004; Yokota et al., 2009). These observations have provided many insights into the terrestrial carbon cycle (Keeling, 1960; Bolin & Keeling, 1963; Bacastow, 1976; Tans et al., 1989; Keeling et al., 1996; Bowman et al., 2017; J. Liu et al., 2017; Chatterjee et al., 2017). However, current measurement programs are unable to continuously monitor CO₂ with global coverage, resulting in observational gaps. These spatial and temporal gaps in observations of atmospheric CO₂ can introduce artifacts into NEE estimates, leading to difficulties in constraining carbon fluxes on regional scales (J. Liu et al., 2014; Byrne et al., 2017; Basu et al., 2018).

Different observing systems have different gaps in the observational coverage. Space-based measurements retrieve atmospheric CO₂ from measurements of reflected sunlight. This results in highly seasonal observational coverage in extratropical regions. Seasonal differences in observational coverage are further exasperated by challenging retrievals over snow (Nassar et al., 2014), and seasonal variations in cloud cover. In contrast, surface-based measurements of atmospheric CO₂ typically have comparatively uniform temporal coverage, but poor spatial coverage. Surface measurements sites most densely cover the northern extratropics (particularly North America and Europe) but have sparse coverage elsewhere (Byrne et al., 2017).

In the northern extratropics, surface-based and space-based atmospheric CO₂ measurements provide complementary observational coverage in space and time, respectively. Yet, few studies have attempted to combine surface-based and space-based atmospheric CO₂ measurements to obtain top down constraints on fluxes across the northern latitudes. Chevallier et al. (2011) found consistency between the surface-air-sample-based
and the TCCON-based inversions, suggesting that flux inversions combining both data sources could be performed. Houweling et al. (2015) performed a series of CO$_2$ flux inversions assimilating measurements from the Greenhouse Gases Observing Satellite (GOSAT) and surface-based CO$_2$ measurements. They found that comparisons between posterior CO$_2$ fields and aircraft data did not show significant differences between inversions assimilating surface-based or space-based measurements, and that the largest differences were driven by the inversion set up. However, they also found that the two datasets gave large differences in the spatial distribution of the CO$_2$ sink, with GOSAT flux inversions having increased uptake in the northern extratropics by $\sim$1 PgC. When both datasets were combined, they found that the posterior fluxes did not recover the observed meridional gradient in CO$_2$ (which was also found for the GOSAT flux inversions), suggesting that the biases in retrieved GOSAT X$_{CO2}$ could be adversely impacting the results.

Another study, Wang et al. (2018), assimilated both GOSAT measurements and surface-based atmospheric CO$_2$ measurements in a batch Bayesian synthesis inversion. They found that the differences in observational coverage of the ground-based and space-based datasets were complementary, resulting in smaller posterior uncertainty estimates when both datasets are assimilated than either dataset alone. Similarly, in a set of regional Observing System Simulation Experiments (OSSEs), Fischer et al. (2017) showed reduced uncertainty in biosphere and fossil fuel emissions in California by combining space-based X$_{CO2}$ and surface-based flask and in situ measurements.

In this study, we further investigate combining ground-based and space-based measurements of atmospheric CO$_2$ to provide estimates of NEE globally, but we focus on northern extra-tropical regions where surface-based and aircraft-based measurements are most densely concentrated. We perform a series of six-year flux inversions (2010–2015, inclusive) assimilating surface-based measurements from the in situ and flask measurement network, TCCON column-averaged dry-air CO$_2$ mole fractions (X$_{CO2}$), GOSAT X$_{CO2}$ measurements, and all three datasets combined. For each set of measurements, we perform three flux inversions applying different prior NEE flux and error constraints. From the spread in posterior fluxes due to prior constraints, we quantify the precision to which these datasets constrain posterior fluxes. Spatial structures in the posterior fluxes are examined through comparisons between posterior-NEE-simulated X$_{CO2}$ and Orbiting Carbon Observatory 2 (OCO-2) X$_{CO2}$ measurements and the accuracy of posterior-NEE-simulated CO$_2$ is examined through comparisons with aircraft-based CO$_2$ measurements.

The paper is outlined as follows. Section 2 describes the measurements used in this study and Sec. 3 describes the flux inversion set-up. The posterior CO$_2$ fields obtained by the flux inversions are compared with OCO-2 and aircraft-based measurements in Sec. 4.1. We then examine the six-year-mean seasonal cycle and annual net fluxes (Sec. 4.2) and interannual variability (Sec. 4.3) obtained by the flux inversions. Finally, the implications of the results are discussed in Sec. 5 and conclusions are given in Sec. 6.

2 Data

2.1 Surface-based in situ and flask measurements

Surface-based measurements of boundary layer atmospheric CO$_2$ can be performed using an in situ gas analyzer or by taking a flask sample, which is then returned to a lab and analyzed. A number of different groups from around the world collect surface CO$_2$ observations. We assimilate measurements from version 4.1 of the GLOBALVIEW plus package (Masarie et al., 2014; Cooperative Global Atmospheric Data Integration Project, 2018) and the Japan-Russia Siberian Tall Tower Inland Observation Network (JR-STATION) of nine tower sites in Siberia (Sasakawa et al., 2010, 2013).

The GLOBALVIEW v4.1 package incorporates data from many observing sites around the world and is specifically prepared for use in data assimilation studies. We include...
measurements from the Integrated Carbon Observation System (ICOS RI, 2019) in our analysis. We assimilate GLOBALVIEW v4.1 measurements from surface in situ and flask sites, tower sites, and ship-based measurements. Data is only assimilated if the measurements are assimilated by NOAA’s CarbonTracker, version CT2017 (CT_assim = 0). Measurements are assimilated at the intake height above the model surface over land, and at the intake height above sea level for ocean grid cells. For surface-based flask and in situ measurements, most of the measurement error applied for assimilation is due to representativeness errors (inability to model these measurements). We use the model-data-mismatch (mdm) as the measurement errors. This is the error value placed on each measurement in the assimilation system, and is meant to express the statistics of simulated-minus-observed CO2 residuals expected if CarbonTracker were using perfect surface fluxes.

JR-STATION is a network of nine towers (http://www.cger.nies.go.jp/en/climate/pj1/tower/). On these towers, high inlet measurements are obtained over the 17–20th minutes of each hour and the low inlet data is obtained from 37–40th minutes of each hour, these 3-minute averages are the taken to be representative of the hourly means for each inlet. We filter the measurements by removing all measurements where the vertical gradient in CO2 exceeds 0.5 ppm (to remove measurements when the boundary layer is not well-mixed), and use the measured value at the highest intake for the measurement. For each site the errors (in ppm) are prescribed to be constant throughout a given month, the errors are the errors range from 3 ppm in winter to 7 ppm in summer, to account for both measurement and representativeness errors. These error estimates were chosen because they are comparable to the error estimates for tower sites in the GLOBALVIEW plus v4.1 package.

We remove outliers and poorly modeled measurements by filtering out measurements for which the difference between the prior-NEE-simulated measurements and actual measurements exceeds three standard deviations of the measurement uncertainty (See Sec. 3 for details on the forward model simulations). We also remove measurements for which the difference between prior simulated CO2 and measurement exceeds 10 ppm, as these are assumed to be poorly simulated by the model. This filtering removes ~8% of the measurements. For each site, the data is only assimilated between 11 a.m. and 4 p.m. local time.

2.2 Aircraft-based measurements

Aircraft measurements are used for the evaluation of posterior atmospheric CO2 fields. Aircraft data are obtained from the version 4.1 of the GLOBALVIEW plus dataset. Comparisons between measured and modeled atmospheric CO2 are performed over three distinct regions: East Asia, North America, and Alaska/Arctic (Fig. S1). Aircraft measurements over East Asia come exclusively from the Comprehensive Observation Network for Trace gases by Airliner (CONTRAIL) program (Machida et al., 2008, 2018). Aircraft data over Alaska/Arctic and North America originate from the NOAA Global Greenhouse Gas Reference Network’s aircraft program (Sweeney et al., 2015) and HIPPO Pole-to-Pole Observations (HIPPO) (Wofsy, 2011). The number of hourly-mean measurements per month between 3–8 km in altitude above sea level (asl) are shown in Fig. S2.

2.3 TCCON measurements

TCCON is a network of ground-based Fourier transform spectrometers that record solar absorption spectra in the near-infrared from which, among other gases, XCO2 is estimated (Wunch et al., 2011). CO2 abundances are retrieved using a non-linear least squares approach from absorption lines in the near-infrared spectral region. The column-averaged dry-air mole fractions of CO2 (XCO2) is calculated by taking the ratio of the column abundance of CO2 to O2 (scaled by the mean O2 concentration), resulting in high precision
Table 1. TCCON sites used in this study.

| Site Name         | Lat     | Lon     | Start Date   | Reference                           |
|-------------------|---------|---------|--------------|-------------------------------------|
| Eureka            | 80.05 N | 86.42 W | 25 Jul 2010  | Strong et al. (2017)                |
| Orleans           | 47.97 N | 2.11 E  | 29 Aug 2009  | Warneke et al. (2017)               |
| Park Falls        | 45.95 N | 90.27 W | 02 Jun 2004  | Wennberg, Roehl, et al. (2017)     |
| Rikubetsu         | 43.46 N | 143.77 E| 16 Nov 2013  | Morino et al. (2017)                |
| Lamont            | 36.60 N | 97.49 W | 06 Jul 2008  | Wennberg, Wunch, et al. (2017)     |
| Edwards           | 34.96 N | 117.88 W| 20 Jul 2013  | Iraci et al. (2017)                 |
| Ascension Island  | 7.92 S  | 14.33 W | 22 May 2012  | Feist et al. (2017)                 |
| Darwin            | 12.46 S | 130.93 E| 28 Aug 2005  | Griffith, Deutscher, et al. (2017)  |
| Reunion Island    | 20.90 S | 55.49 E | 16 Sep 2011  | De Mazière et al. (2017)            |
| Wollongong        | 34.41 S | 150.88 E| 26 Jun 2008  | Griffith, Velazco, et al. (2017)    |

(<0.25% in CO₂) X\textsubscript{CO}_2 measurements. The TCCON strives to achieve the best site-to-site precision and accuracy possible. Systematic biases that are consistent throughout the network are fully accounted for by scaling the TCCON retrieval results to the WMO scale via aircraft and AirCore profiles (Wunch et al., 2010). Moreover, the TCCON sets guidelines to ensure that the instrumentation at each site is as similar as possible, and that the retrieval software, including the spectroscopic line lists and line shapes, is identical for each site. However, site-specific differences (e.g. instrumental line shape) can cause residual site-to-site biases (Wunch et al., 2010) which might introduce biases in flux inversions.

For this study, TCCON data were obtained from the TCCON Data Archive, hosted by CaltechDATA [https://tccondata.org]. We include data from TCCON sites that have mean biases of less than 0.5 ppm relative to both the OCO-2 target-mode X\textsubscript{CO}_2 and the posterior-simulated X\textsubscript{CO}_2 from the surface-only flux inversions. The sites included in this study, which provide data during the years 2010–2015, are given in Table 1. Sites that are excluded from this study are excluded due to several factors that cause apparent biases to be greater than 0.5 ppm. These factors include: proximity to large CO₂ sources (e.g., cities), proximity to large topographic variability, and in a few cases, known TCCON instrument biases for which a solution either has been applied, or will be applied in an upcoming TCCON data version. Note that the threshold of 0.5 ppm is somewhat arbitrary. This value was set because most sites outside of this threshold are in heavily observed regions (e.g., Europe), which are expected to be well constrained by other datasets (Byrne et al., 2017), or in the Southern Hemisphere and not expected to have a large impact on the performance of the flux inversions in the northern mid-latitudes.

In this study, the TCCON data are filtered to remove measurements with solar zenith angles greater than 70 degrees. Measurements are then binned into hourly medians for each site. Only hours with five or more measurements are included. Measurements are only assimilated between 11am-3pm local time for the flux inversions, to minimize potential biases relating to errors in the prescribed diurnal cycle of NEE.

2.4 Space-based measurements

We assimilate X\textsubscript{CO}_2 measured by the Thermal And Near-infrared Sensor for carbon Observations Fourier Transform Spectrometer (TANSO-FTS) aboard GOSAT. GOSAT was launched in February 2009 in a sun-synchronous orbit, with a repeat cycle of 3 days that produces 44 separate ground track repeats (Yoshida et al., 2013). The footprint of the GOSAT measurements has a diameter of about 10 km. Since August 2010, TANSO-FTS has been measuring with a 3-point cross-track pattern with 263 km cross track separation, resulting in a swath of 526 km. Measurements have an along-track separation
of 283 km (Crisp et al., 2012). We use version 7.3 of the NASA Atmospheric CO\textsubscript{2} Observations from Space (ACOS) GOSAT measurements in this analysis. A detailed description of ACOS retrieval algorithm is available in O’Dell et al. (2012) and Crisp et al. (2012), with recent updates described in Eldering et al. (2017) and O’Dell et al. (2018). We assimilate all high gain (H-Gain) nadir measurements from the TANSO-FTS shortwave infrared (SWIR) band that pass the quality flag requirement.

Measurements from OCO-2 are used for comparisons with the posterior CO\textsubscript{2} fields. OCO-2, launched in July 2014, is a space-based spectrometer in a Sun-synchronous orbit that measures reflected solar radiation to infer X\textsubscript{CO\textsubscript{2}} with a footprint of about 3 km\textsuperscript{2}. It has a repeat cycle of 16 days, resulting in 233 separate ground track repeats. OCO-2 has a swath of 10 km and collects eight adjacent, spatially resolved samples every 0.333 s, resulting in roughly 24 soundings per second. We downloaded version 9 of the ACOS OCO-2 lite files from the CO\textsubscript{2} Virtual Science Data Environment (https://co2.jpl.nasa.gov/). Measurements are averaged into super-obs at 1°×1° resolution grids following J. Liu et al. (2017), with the additional requirement that there must be a minimum of eight OCO-2 observations within each 1°×1° gridbox. We combine land nadir and land glint measurements for the analysis.

3 Flux inversions

Flux inversions are performed with the Greenhouse Gas Framework – Flux (GHGF-Flux) inversion system. GHGF-Flux is a flux inversion system developed under the NASA’s Carbon Monitoring System (CMS) project. The GHGF is capable of jointly assimilating multi-platform observations of CH\textsubscript{4}, CO, CO\textsubscript{2}, and OCS. The GHGF inherits the chemistry transport model from the GEOS-Chem and the adjoint analysis methods from the GEOS-Chem-adjoint.

Chemical transport is driven by the Modern-Era Retrospective Analysis for Research and Applications, Version 2 (MERRA-2) meteorology produced with version 5.12.4 of the GEOS atmospheric data assimilation system (Gelaro et al., 2017). To perform tracer transport, these fields are regridded to 4°×5° horizontal resolution and archived with a temporal resolution of 6 h except for surface quantities and mixing depths, which have a temporal resolution of 3 h. Tracer transport is performed at 30 min time steps.

For all inversions, we optimize 14 day scaling factors for daily net NEE and ocean fluxes, except for the final temporal grouping of each year, which is padded with 1–2 days so that the groupings cover the same day-of-year increments for each year. We use an assimilation window of approximately 18 months (October 7 to April 1 two years later) and keep posterior fluxes for one year (Jan 1 to Dec 31) then shift the inversion window forward one year. Using this method, we optimize NEE spanning 2010–2015. Initial conditions are generated by performing a two year inversion of surface in situ and flask measurements spanning 1 Jan 2008 to 31 Dec 2009. The stratosphere is then adjusted to match the zonal mean structure of Diallo et al. (2017) for October 2009 (adjusted by a few parts per million).

Prior NEE fluxes and errors differ between inversions, and are generated from three different models: the Simple Biosphere model (SiB3), the Carnegie-Ames-Stanford Approach model (CASA) and FLUXCOM. The motivation for using three different priors is that the posterior flux estimates may be sensitive to prior fluxes (Philip et al., 2019), thus using an ensemble of prior flux estimates provides an estimate of the precision to which the observations constrain fluxes. For all prior fluxes the annual total net flux has been adjusted to 4.6 PgC yr\textsuperscript{−1}, to match the mean atmospheric CO\textsubscript{2} growth rate. Details on the modeled NEE fluxes and prior errors are given in Appendix 7. The diurnal cycle in NEE is prescribed using the modeled diurnal cycle from SiB3 for the SiB3 flux inversions and the diurnal cycle from CASA for the CASA and FLUXCOM inversions.
Sensitivity tests found that the flux inversions were not sensitive to the prescribed diurnal NEE cycle. The ECCO-Darwin-V1 model (Menemenlis et al., 2008; Dutkiewicz et al., 2009; Brix et al., 2015) estimates are used as the prior ocean CO$_2$ exchange for all inversions, and prior errors were taken to be 100% of the flux. Fossil fuel, biofuel, and biomass burning CO$_2$ emissions are prescribed using the Open-source Data Inventory for Anthropogenic CO$_2$, version 2018 (Oda & Maksyutov, 2011; Oda et al., 2018) with downscaling to hourly emissions based on Nassar et al. (2013), CASA-GFED4-FUEL, and Global Fire Emission Database, version 4 (GFED4) (Randerson et al., 2018) inventories, respectively.

Prior error covariance matrices are taken to be diagonal, such that there are no spatial or temporal covariances. The prior NEE errors are generated based on the NEE fluxes provided by the models. It is first taken to be 60% of the NEE flux. This is then increased by scaling up the errors at times and grid cells that have active vegetation but small net fluxes. For example, the uncertainty is scaled up during the spring (source to sink) and fall (sink to source) transition periods when the 14-day NEE flux is small but the summer 14-day NEE fluxes are much larger. We also inflate the uncertainty for gridcells in which the flux is small for a given model but is much larger for the other models. The final errors range from 100% to 500% of the NEE flux. Additional details are provided in Appendix 7.

A series of flux inversions are performed that assimilate different datasets. This allows us to quantify the influence of different observational datasets on the posterior fluxes. We perform flux inversions that assimilate only ground-based in situ and flask measurements (referred to as surface-only), only TCCON measurements (TCCON-only), only GOSAT data (referred to as GOSAT-only), and all datasets simultaneously (referred to as GOSAT+surface+TCCON). For each data assimilation set-up, we perform flux inversions with each of the three prior NEE fluxes and errors. Therefore, we perform a total of 12 flux inversions.

### 4 Results

#### 4.1 Evaluation of posterior-NEE-simulated CO$_2$

Large spatial structures in the posterior-simulated CO$_2$ fields are compared with GOSAT and OCO-2 X$_{CO_2}$, while the accuracy of the fluxes are evaluated against aircraft-based CO$_2$ measurements. Rather than describing the data–model differences for all 12 inversions, the posterior fluxes are grouped by the dataset assimilated and the mean posterior fluxes are evaluated. Tables giving the data–model mismatch between the individual flux inversions and aircraft measurements are provided as supplementary materials (Tables SS1 and SS2).

#### 4.1.1 Comparison of posterior CO$_2$ against space-based X$_{CO_2}$

Space-based X$_{CO_2}$ measurements have broad spatial coverage on the timescale of a month. This allows for comparisons between modeled and measured X$_{CO_2}$ data over large spatial scales. Here, the data–model mismatch between the posterior CO$_2$ fields and space-based measurements from GOSAT and OCO-2 are examined. Figure 1 shows the zonal mean data–model mismatch as a function of latitude and time for the mean prior fluxes and mean posterior fluxes for the TCCON-only inversions, surface-only inversions, GOSAT-only inversions, and GOSAT+surface+TCCON inversions. Note that there are gaps due to GOSAT’s observational coverage in the tropics and at high latitudes. The mean prior flux gives larger data–model standard deviations against GOSAT (0.59 ppm) and OCO-2 (0.67 ppm) than all of the flux inversions, implying that the flux inversions improve the variance of the data–model mismatch. The CO$_2$ fields simulated with the prior fluxes tend to be biased low relative to GOSAT and OCO-2 during the
winter and spring and biased high during the summer and fall in the northern extratropics, suggesting that the prior fluxes underestimate the magnitude of the seasonal cycle. Comparing the posterior CO\textsubscript{2} fields against GOSAT, the surface-only and TCCON-only flux inversions give the largest mean data–model standard deviations, which is expected as there were the only inversions that do not assimilate GOSAT data.

Comparing to OCO-2, all of the flux inversions give similar differences. Mean differences range from -0.11 ppm to 0.07 ppm and standard deviations range over 0.41-0.48 ppm, suggesting that all of the flux inversions recover the global X\textsubscript{CO\textsubscript{2}} fields with similar accuracy and precision. However, north of 40 \degree N, the GOSAT+surface+TCCON flux inversion shows better agreement with OCO-2 (RMS=0.30 ppm) than the other flux inversions (RMS=0.36-0.41 ppm). Differences between posterior-simulated X\textsubscript{CO\textsubscript{2}} and the OCO-2 measurements are largest in the northern subtropics, where the assimilated datasets have sparse observational coverage. Thus, it is unclear whether the differences in the subtropics are due to gaps in the observational coverage or biases in the OCO-2 retrievals.

4.1.2 Evaluation of posterior CO\textsubscript{2} against aircraft-based measurements

Aircraft-based measurements of atmospheric CO\textsubscript{2} provide a constraint on atmospheric CO\textsubscript{2} that is independent of the surface-based and space-based datasets assimilated. Therefore, aircraft-based CO\textsubscript{2} measurements offer a dataset that modeled atmospheric CO\textsubscript{2} can be evaluated against. Here, we evaluate the atmospheric CO\textsubscript{2} fields simulated using the prior and posterior fluxes against aircraft measurements over three regions with intensive sampling: East Asia, North America, and Alaska/Arctic. We only use aircraft data between 3–8 km in altitude above sea level. Differences between measured and modeled CO\textsubscript{2} are due to both model transport errors and surface flux errors. We have found that the differences are strongly influenced by model transport errors for individual measurements but that the impact of representativeness errors on data–model mismatches is reduced with temporal aggregation, thus we aggregate data–model mismatches to monthly means.

The GOSAT+surface+TCCON flux inversions generally show the best agreement with the aircraft-based CO\textsubscript{2} measurements. Figure 3 shows the monthly-mean aircraft measurements and modeled CO\textsubscript{2} for the three regions examined here. The GOSAT+surface+TCCON flux inversions give the smallest RMS difference against aircraft-based CO\textsubscript{2} in East Asia.
Figure 1. Zonal mean data–model mismatch for space-based XCO₂ measurements as a function of latitude and time for the (a) prior fluxes, (b) TCCON-only inversions (c) surface-only inversions, (d) GOSAT-only inversions, and (e) GOSAT+surface+TCCON inversions. For each set of flux inversions, the three panels show (i) the zonal and monthly mean GOSAT XCO₂ data–model difference for 2010 through 2015. (ii) The mean GOSAT XCO₂ data–model difference for each month of the year. (iii) The zonal and monthly mean OCO-2 XCO₂ data–model difference for 2014 through 2015.
Figure 2. Spread in zonal and monthly mean simulated GOSAT X\textsubscript{CO2} for (a) prior NEE, (b) TCCON-only, (c) surface-only posterior NEE, (d) GOSAT-only posterior NEE, (e) GOSAT+surface+TCCON posterior NEE as a function of latitude and time. For each set of flux inversions sets, the panels show (i) the zonal and monthly mean range for 2010 through 2015, and (ii) The mean range for each month of the year.
Figure 3. Comparison of monthly mean measured and simulated aircraft-based CO$_2$ for (a) East Asia, (b) North America, and (c) Alaska/Arctic. For each region, the mismatch for (left to right) prior, TCCON-only, surface-only, GOSAT-only, and GOSAT+surface+TCCON simulated CO$_2$ are shown. The top panel shows a scatter plot of the simulated aircraft-based CO$_2$ against the measured aircraft-based CO$_2$, and the error bars indicate the spread in posterior NEE. The lower panel shows the mean data–model mismatch for each month, with error bars showing the range of monthly mean mismatched over the six-years and inversion set-ups. Colors correspond to the month of year.

(0.35 ppm) and North America (0.50 ppm). The GOSAT-only flux inversions give the smallest RMS difference over the Alaska/Arctic region (0.79 ppm), although all of the flux inversions give larger RMS differences over this region relative to the midlatitude regions, suggesting that none of the flux inversions fully recover NEE at high latitudes. These aircraft measurements are also sensitive to fluxes over Siberia (Fig. S4), which is poorly observed by all datasets. Differences in the data–model mismatch between flux inversions are evident as a function of month-of-year. The GOSAT+surface+TCCON flux inversion tends to best capture month-to-month variability, while both flux inversions assimilating GOSAT measurements tend to have less seasonality in the data–model mismatch than the TCCON-only and surface-only flux inversions. This is most evident for East Asia and suggests that the GOSAT-only flux inversions better capture the month-to-month variability in fluxes (consistent with the results of Polavarapu et al. (2018) and Byrne et al. (2019)).

Despite these differences, the data–model biases against the aircraft-based measurements are generally similar between flux inversions. For example, all of the flux in-
versions give positive biases for East Asia (0.12–0.30 ppm) and North America (0.38–
0.47 ppm) but negative biases for the Alaska/Arctic region (-0.07 to -0.03 ppm). The
fact that the data–model biases are similar suggests that these biases are sensitive to trans-
port errors. This was quantified by regridding the fluxes and performing the evaluation
against aircraft measurements at 2°×2.5° spatial resolution (Figure S3). We find that
model-data biases for the flux inversions change by 0.01–0.03 ppm for East Asia, 0.07–
0.10 ppm for North America, and 0.08–0.11 ppm for Alaska/Arctic. These differences
are similar to the magnitude of data–model differences between flux inversions, suggest-
ing that transport model errors limit the ability of evaluating CO₂ flux estimates with
aircraft-based measurements.

4.2 Mean fluxes

4.2.1 Seasonal Cycle

In the northern extratropics, the seasonal cycle of NEE produces a large annual
oscillation in atmospheric CO₂, giving seasonal variations of ~10 ppm in XCO₂. This pro-
vides the largest signal of ecosystem carbon dynamics in atmospheric CO₂ and is the NEE
signal that is best captured in CO₂ flux inversions. In this section, we examine the sea-
sonal cycle of NEE recovered by the flux inversions in the northern extratropics grouped
by the assimilated dataset. Figure 5 shows the seasonal cycle for the entire northern ex-
tratropics and five sub-continental regions (the spatial extent of the sub-continental re-
regions are shown in Fig. 4). We examine (1) the consistency in the seasonal cycle between
the datasets and (2) the precision of the posterior fluxes due to prior assumptions.

The posterior seasonal cycles of the flux inversions show consistent seasonal cycles
for all assimilated datasets, relative to the prior fluxes. The GOSAT+surface+TCCON
NEE fluxes most closely match the GOSAT-only NEE fluxes during the summer, as GOSAT
has dense observational coverage. During the winter, the GOSAT+surface+TCCON NEE
fluxes most closely match the surface-only fluxes, particularly over temperate North Amer-
ica and Europe where the surface-based measurements are most densely concentrated.

The spread for each set of flux inversions shows the range in posterior fluxes due
to differences in the prior fluxes and errors applied. This provides a metric of the pre-
Figure 5. Prior and posterior NEE fluxes for (a) the entire northern extratropics (≥30° N), (b) temperate North America, (c) northern North America, (d) Europe, (e) east Asia, and (f) north Asia at 14 day temporal resolution. The shaded curves show the range of posterior fluxes obtained by the GOSAT-only (purple), TCCON-only (grey), surface-only (yellow), and GOSAT+surface+TCCON (dark green) flux inversions. Dashed lines show the seasonal cycles for the three prior NEE fluxes used in inversions: SiB3 (green), CASA (blue), and FLUXCOM (red).

4.2.2 Annual net fluxes

Here, we examine the annual net fluxes obtained for the flux inversions over the northern extratropics. Figure 6 shows the six-year mean annual net fluxes for each subcontinental region. Over the entire northern extratropics (>30° N), the flux inversions show high consistency relative to the spread in the prior. We obtain a mean annual net flux of $-2.80 \text{ PgC yr}^{-1}$ (range of $-3.43$ to $-2.41 \text{ PgC yr}^{-1}$) for the TCCON-only flux inversions, $-2.76 \text{ PgC yr}^{-1}$ (range of $-3.20$ to $-2.49 \text{ PgC yr}^{-1}$) for the surface-only flux inversions, $-2.89 \text{ PgC yr}^{-1}$ (range of $-3.31$ to $-2.65 \text{ PgC yr}^{-1}$) for the GOSAT-only flux inversions, and $-3.02 \text{ PgC yr}^{-1}$ (range of $-3.21$ to $-2.89 \text{ PgC yr}^{-1}$) for the GOSAT+surface+TCCON flux inversions. It is notable that the prior assumptions applied to the flux inversions introduce substantial differences into the posterior fluxes. The range in the northern extratropical sink due to applying different prior NEE fluxes and errors is $0.32$–$1.03 \text{ PgC yr}^{-1}$, depending on the assimilated dataset.
On regional scales, there is generally overlap in the range of net annual fluxes between the TCCON-only, surface-only, GOSAT-only, and GOSAT+surface+TCCON flux inversions. This suggests that these observational datasets provide a consistent constraint on regional net annual NEE, within the considerable uncertainty introduced through prior assumptions. The exception is north Asia, where the surface-only inversions suggest a systematically larger sink than the GOSAT-only flux inversions. This region has poor observational coverage, which may explain the differences seen here.

4.3 Interannual variability

Interannual variability (IAV) in NEE provides a measure of the response of ecosystems to climate variability. Here, we examine the IAV recovered by the flux inversions, where IAV is calculated to be the anomaly from the six-year mean. Figure 7 shows the IAV in NEE for the entire northern extratropics and five extratropical regions at 14-day temporal resolution, after performing a 3-point (42-day) running mean to filter out high frequency variability. The posterior NEE IAV is not sensitive to the prior NEE constraints applied in the flux inversion, such that similar posterior NEE IAV is recovered for each set of prior fluxes when a given assimilated dataset. This is illustrated by the small range obtained for each set of colored curves. However, the posterior NEE IAV is sensitive to the assimilated dataset, such that we find disagreement in NEE IAV for the TCCON-only, surface-only, and GOSAT-only flux inversions.

Differences in IAV between flux inversions can partially be explained by differences in the observational coverage of the datasets. As an example, let’s consider the differences in IAV between the surface-only and GOSAT-only flux inversions in 2011 over temperate North America (Fig. 8). Figure 8a shows the monthly CO$_2$ anomalies observed by GOSAT and the surface in situ and flask network over the summer of 2011. GOSAT X$_{CO2}$ measurements are distributed uniformly across North America, while surface in situ and flask measurements are located south of Lake Superior. This observational coverage is reflected in the posterior fluxes. The GOSAT-only posterior NEE anomalies (Fig. 8b) reflect the large scale structures in the X$_{CO2}$ anomalies but miss smaller scale structures, such as the positive anomalies over south central North America. The surface-only posterior anomalies (Fig. 8c) capture large anomalies seen in CO$_2$, such as the anomalous release of CO$_2$ in south central North America, but miss much of the large scale structures. Combining these two datasets in a single inversion, referred to as “GOSAT+surface”, captures both the large scale structures from the GOSAT-only and small-scale structures from the surface-only flux inversion (Fig. 8d). The posterior NEE anomalies from the
Figure 7. IAV in NEE for 2010–2015 at 14 day temporal resolution for (a) the entire northern extratropics (\(\geq 30^\circ\) N), (b) temperate North America, (c) northern North America, (d) Europe, (e) east Asia, and (f) north Asia. The shaded curves show the range of posterior fluxes obtained by the GOSAT-only (purple), TCCON-only (grey), surface-only (yellow), and GOSAT+surface+TCCON (dark green) flux inversions. A 3-point (42 day) running mean is performed to remove high frequency variability.
GOSAT+surface flux inversion also correlate with anomalies in soil temperature (mean of MERRA-2 soil temperature over levels 1–3, Reichle et al. (2011, 2017)) (Fig. 8e) and soil moisture (ESA CCI Surface Soil Moisture Product, Y. Y. Liu et al. (2011, 2012); Wagner et al. (2012); Gruber et al. (2017); Dorigo et al. (2017)) (Fig. 8f) over this time period, suggesting that combining these datasets produces more realistic NEE IAV. Similar results were found over Eurasia during the summer of 2010 (Fig. S5).

On an annual basis, we find mixed agreement between flux inversions in year-to-year variations. Figure 9 shows IAV in annual net NEE anomalies for the entire northern extratropics. In general, IAV in annual net fluxes are consistent for a given set of assimilated data, suggesting that the results are not sensitive to the prior fluxes and errors used. Note that the prior NEE fluxes did not contain IAV, which has previously been shown to have a substantial impact on posterior NEE IAV (Byrne et al., 2019). However, posterior IAV is quite variable between different assimilated datasets. The cause of these differences between the flux inversions is likely partially due to differences in the observational coverage between datasets. It is possible that differences between datasets are also partially due to changes in the observational coverage over time, which has previously been shown to have an impact on inferred fluxes (Rödenbeck et al., 2003; Gurney et al., 2008; Bruhwiler et al., 2011).

5 Discussion

5.1 Consistency in surface-based and spaced-based flux constraints

The results generally show good agreement between the flux inversions assimilating different datasets. The agreement between the surface-only and GOSAT-only flux inversions may seem surprising in the context of a number of previous studies that have shown substantial differences between surface-based and space-based flux estimates (Basu et al., 2013; Chevallier et al., 2014; Houweling et al., 2015). However, more recent studies have shown improved agreement between surface-based and space-based flux inversions. Chevallier et al. (2019) found that flux inversions assimilating OCO-2 ACOS version 9 measurements gave similar net annual fluxes to those assimilating surface-based measurements, and that both compared well against aircraft measurements. Interestingly, Chevallier et al. (2019) also found that GOSAT OCO Full Physics (OCFP) v7.1 XCO₂ retrievals did not compare as well against aircraft measurements. Comparisons between the ACOS 7.3 and OCFP v7.1 (downloaded from the Copernicus Climate Change Service, https://climate.copernicus.eu/) show substantial differences in zonal mean XCO₂ (Fig. S6). Furthermore, GOSAT ACOS 7.3 retrievals are found to give better agreement with posterior-simulated-CO₂ from the surface-only flux inversion (Fig. S7). This suggests that the specific retrieval algorithm used has a large impact on the posterior fluxes, such that the improved agreement between surface-based and space-based measurements found in recent studies may be primarily due to improvements in the ACOS XCO₂ retrieval algorithm. Miller and Michalak (2019) have also argued that recent improvements in the ACOS algorithm have substantially increased the reliability of OCO-2 XCO₂ measurements in flux inversions studies (for version 8 in particular). Substantial work has gone into refining the ACOS retrieval algorithm over the past decade (O’Dell et al., 2012; Crisp et al., 2012; Eldering et al., 2017; O’Dell et al., 2018; Kiel et al., 2019; Nelson & O’Dell, 2019). Thus, the improved agreement between surface-based and space-based CO₂ constraints is likely best explained by improvements in the ACOS retrieval algorithm.

A consistent six-year mean northern extratropical sink is obtained by all observational datasets. This result is in contrast to several previous studies that found substantial differences in the annual net NEE flux of CO₂ in the northern extratropics between flux inversions assimilating surface-based and space-based measurements (Basu et al., 2013; Saeki et al., 2013; Chevallier et al., 2014; Reuter et al., 2014). The reason why we obtain a more consistent annual net flux between datasets than some earlier studies is
Figure 8. Monthly anomalies in (a) GOSAT $X_{\text{CO}_2}$ (ppm, $4^\circ \times 5^\circ$ grid cells) and surface site CO$_2$ (ppm divided by four, circles), (b) GOSAT-only posterior NEE, (c) surface-only posterior NEE, (d) GOSAT+surface posterior NEE, (e) MERRA-2 soil temperature, (f) ESA CCI soil moisture, for (left-to-right) May, June, and July of 2011.
Figure 9. Annual net IAV in NEE over 2010-2015 for the TCCON-only, surface-only, GOSAT-only, and GOSAT+surface+TCCON flux inversions. Shaded grey regions show the range for the fluxes, while the solid black line shows the mean. Individual inversions are shown by the filled circles, with colors indicating prior NEE applied: green circles indicate SiB3, blue circles indicate CASA, and red circles indicate FLUXCOM.

not immediately clear, but could be due to advancements in the retrieval algorithm (e.g., ACOS 3.3 and earlier versions were used in Houweling et al. (2015)) or due to the fact that we look at a multi-year mean while earlier studies looked at shorter time periods (e.g., Houweling et al. (2015) only examined June 2009 to June 2010). In fact, we find that the surface-only inversion suggests weaker uptake in 2010 than average (by 0.40 to 0.49 PgC yr\(^{-1}\)), while the GOSAT flux inversion suggests near average uptake (see Sec. 4.3), suggesting that the difference in inferred fluxes between these two datasets may have been unusually large for 2010. However, it is important to note that differences in annual net fluxes do not imply biases in the measurements. There are aspects of the inversion setups that can lead to differences. For example, differences in the distribution of observations can lead to significant differences in annual net fluxes (J. Liu et al., 2014; Byrne et al., 2017; Basu et al., 2018). Thus, one should not necessarily expect consistent annual net fluxes from observational datasets with spatial and temporal gaps in observational coverage.

5.2 Does combining datasets improve flux inversions?

Is it possible to conclude that the GOSAT+surface+TCCON flux inversions improve flux estimates relative to the flux inversions that assimilate a single dataset? Of course, the answer to this question depends on how “improve” is defined. The GOSAT+surface+TCCON flux inversions generally show a small reduction in model-data differences against independent aircraft-based CO\(_2\) and OCO-2 X\(_{CO_2}\) (north of 40°N). This suggests that combining these datasets in a flux inversion framework produces NEE fluxes that better recover the true atmospheric CO\(_2\) fields than any dataset alone. However, confounding factors in evaluating these fluxes remain a significant concern. Model transport errors appear to be a main driver of data-model differences for aircraft-based CO\(_2\) measurements, and obscures the source of data-model differences. Evaluating optimized fluxes against OCO-2 is also problematic because these retrievals are known to have their own biases.

The GOSAT+surface+TCCON flux inversions improve the precision of the posterior NEE fluxes relative to the flux inversions assimilating one dataset. This is found to be the case at seasonal, annual, and interannual scales. The GOSAT+surface+TCCON flux inversions closely resemble the GOSAT-only NEE fluxes during the summer and surface-only fluxes during the winter for five northern extratropical regions. This is expected given the spatiotemporal distribution of GOSAT and surface-based CO\(_2\) measurements and suggests that the GOSAT+surface+TCCON posterior NEE fluxes are better constrained.
by the observations than the GOSAT-only or surface-only flux inversions. Therefore, the
GOSAT+surface+TCCON flux inversions are less likely to be impacted by biases in the
observational coverage, such that, from an observational coverage perspective, we can
conclude that the GOSAT+surface+TCCON flux inversions are better constrained than
the GOSAT-only or surface-only flux inversions.

An important concern in combining CO\textsubscript{2} datasets within a single flux inversion sys-
tem is that there could be relative biases in the atmospheric CO\textsubscript{2} constraints provided
by the different datasets. Any inconsistency in flux constraints between datasets has the
potential of introducing artifacts into the posterior fluxes. Biases in the observations could
be present due to errors in the X\textsubscript{CO\textsubscript{2}} retrieval algorithm, representativeness errors (Agustí-
Panareda et al., 2019) or model transport errors. Several previous studies have suggested
that unrealistically large uptake over Europe (\textasciitilde 1.5 PgC yr\textsuperscript{-1}) is recovered in posterior
fluxes due to biases in the GOSAT retrieval algorithm (Basu et al., 2013; Chevallier et
al., 2014), although the ACOS retrieval algorithm has undergone significant development
since these studies (Eldering et al., 2017; O’Dell et al., 2018) resulting in reduced biases
(Miller & Michalak, 2019). Similarly, a number of studies have pointed out systematic
transport errors in GEOS-Chem (Yu et al., 2018; Schuh et al., 2019), as well as biases
in reanalysis winds (e.g., vertical mixing, Parazoo et al. (2012)). We do not find clear
evidence for biases between the surface-based and GOSAT constraints, although, these
biases may be challenging to identify. However, we do see the impact of model transport
errors in comparisons between the posterior-simulated-CO\textsubscript{2} and aircraft measurements.
Ideally, this analysis should be performed with two different transport models so that
transport related errors could be more easily identified.

6 Conclusions

This study presented a series of flux inversions assimilating surface-based flask and
in situ CO\textsubscript{2} measurements, TCCON X\textsubscript{CO\textsubscript{2}}, GOSAT X\textsubscript{CO\textsubscript{2}}, or all datasets combined. All
of the flux inversions showed improved agreement with independent aircraft-based CO\textsubscript{2}
measurements relative to prior flux estimates. The GOSAT+surface+TCCON flux in-
version gave the smallest RMS differences against aircraft-based CO\textsubscript{2} measurements over
East Asia and North America, and OCO-2 X\textsubscript{CO\textsubscript{2}} measurements (north of 40° N), sug-
gesting that combining the datasets improves flux estimates. However, the data–model
mismatches were strongly impacted by transport model, which makes robust evaluations
of posterior surface fluxes challenging.

We found that all observing systems generally give consistent posterior NEE fluxes
relative to the spread in prior fluxes. This suggests that these datasets provide consist-
tent information on NEE. The GOSAT+surface+TCCON posterior NEE most closely
resembles the GOSAT-only posterior NEE during the summer and surface-only poste-
rior NEE during the winter, consistent with the temporal variations in the observational
constraints. This suggests that the GOSAT+surface+TCCON flux inversions benefit from
the improved spatiotemporal distribution of measurements, providing posterior fluxes
that are better informed by measurements throughout the year.

The results of this study suggest that surface-based and space-based atmospheric
CO\textsubscript{2} constraints provide consistent constraints on NEE fluxes, and can be combined in
a flux inversion framework. This result stands in contrast to earlier attempts to com-
bine these datasets (Houweling et al., 2015), and suggests that the improved consistency
between the datasets has been made possible by the considerable effort spent refining
the ACOS retrieval algorithm (Eldering et al., 2017; O’Dell et al., 2018; Kiel et al., 2019;
Chevallier et al., 2019; Miller & Michalak, 2019).
7 Appendix: Prior NEE fluxes and errors

7.1 Simple biosphere model (SiB3)

SiB3 was originally designed as a lower boundary for General Circulation Models with explicit treatment of biophysical processes. The ability to ingest satellite phenology was later introduced (P. Sellers et al. (1996); P. J. Sellers et al., 1996), and further refinements included a prognostic canopy air space (Vidale & Stöckli, 2005), more realistic soil and snow (I. Baker et al., 2003) and modifications to calculations of root water uptake and soil water stress (I. Baker et al., 2008). The current version is called SiB3. Simulations used in this analysis use phenology (Leaf Area Index, LAI; fraction of Photosynthetically Active Radiation, fPAR) from the Moderate Resolution Imaging Spectroradiometer (MODIS). MERRA reanalysis is used as model inputs, with precipitation scaled to Global Precipitation Climatology Project (GPCP: Adler et al. (2003)) following I. T. Baker et al. (2010).

These fluxes are adjusted to obtain a global net drawdown equal to 4.6 PgC yr$^{-1}$. To do this, the annual net flux at each grid cell and global total annual net drawdown are calculated. The annual net flux at each grid cell is then scaled so that the annual net flux is 4.6 PgC yr$^{-1}$. The difference between the original and scaled annual net flux at each grid cell is then calculated. From this difference, an adjustment at each grid cell for each 14-day period is performed so that the annual net flux then equals the scaled annual net flux at each grid cell.

The prior NEE errors are generated based on the NEE fluxes provided by the models. It is first taken to be 60% of the NEE flux. This is then increased by scaling up the errors if the mean flux for a given grid cell is large but the flux is small at a given time. For example, the uncertainty is scaled up during the fall. We also inflate the uncertainty where the flux is small for SiB3 but large for CASA and FLUXCOM. The final errors range from 100% to 500% of the NEE flux.

7.2 CASA

The version of the model used here, CASA-GFED3, was modified from Potter et al. (1993) as described in Randerson et al. (1996) and van der Werf et al. (2006). It is driven by MERRA reanalysis and satellite-observed NDVI to track plant phenology. We use the same fluxes as are used for the CarbonTracker 2016 (https://www.esrl.noaa.gov/gmd/ccgg/carbontracker/) prior. CASA outputs monthly fluxes of Net Primary Productivity (NPP) and heterotrophic respiration ($R_H$). From these fluxes, GPP and ecosystem respiration ($R_e$) are estimated to be $GPP = 2NPP$ and $R_e = R_H - NPP$. Temporal downscaling and smoothing was performed from monthly CASA fluxes to 90-min fluxes using temperature and shortwave radiation from the ECMWF ERA-interim reanalysis (note this method differs from Olsen and Randerson (2004). GFED CMS is used for global fire emissions (http://nacp-files.nacarbon.org/nacp-kawa-01/). We use average model fluxes by averaging the fluxes for 2007–2012.

These fluxes are adjusted to obtain a global net drawdown equal to 4.6 PgC yr$^{-1}$. To do this, the annual net flux at each grid cell and global total annual net drawdown are calculated. The annual net flux at each grid cell is then scaled so that the annual net flux is 4.6 PgC yr$^{-1}$. The difference between the original and scaled annual net flux at each grid cell is then calculated. From this difference, an adjustment at each grid cell for each 14-day period is performed so that the annual net flux then equals the scaled annual net flux at each grid cell.

The prior NEE errors are generated based on the NEE fluxes provided by the models. It is first taken to be 60% of the NEE flux. This is then increased by scaling up the errors if the mean flux for a given grid cell is large but the flux is small at a given time. For example, the uncertainty is scaled up during the fall. We also inflate the uncertainty...
where the flux is small for CASA but large for SiB3 and FLUXCOM. The final errors range from 100% to 500% of the NEE flux.

### 7.3 FLUXCOM

FLUXCOM products are generated using upscaling approaches based on machine learning methods that integrate FLUXNET site level observations, satellite remote sensing, and meteorological data (Tramontana et al., 2016; Jung et al., 2017). Jung et al. (2017) generate $R_e$ products using several machine learning methods. For this study, we downloaded the products generated using random forests (RF), multivariate regression splines (MARS) and artificial neural networks (ANN) at daily resolution from the Data Portal of the Max Planck Institute for Biochemistry (https://www.bgc-jena.mpg.de). The mean seasonal cycle over 2008-2012 is calculated for each product.

These fluxes are adjusted to obtain a global net drawdown equal to 4.6 PgC yr$^{-1}$. For FLUXCOM, we only adjust fluxes south of 35° N because the northern extratropical NEE fluxes have been heavily informed by FLUXNET sites. For grid cells south of 35° N, the annual net flux at each grid cell and global total annual net drawdown are calculated. The annual net flux at each grid cell is then scaled so that the annual net flux is 4.6 PgC yr$^{-1}$. The difference between the original and scaled annual net flux at each grid cell is then calculated. From this difference, an adjustment at each grid cell for each 14-day period is performed so that the annual net flux then equals the scaled annual net flux at each grid cell.

The prior NEE errors are generated based on the NEE fluxes provided by the models. It is first taken to be 60% of the NEE flux. This is then increased by scaling up the errors if the mean flux for a given gridcell is large but the flux is small at a given time. For example, the uncertainty is scaled up during the fall. We also inflate the uncertainty where the flux is small for FLUXCOM but large for SiB3 and CASA. The final errors range from 100% to 500% of the NEE flux.

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Supporting Information for “Improved constraints on northern extratropical CO₂ fluxes obtained by combining surface-based and space-based atmospheric CO₂ measurements”

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2. Tables S1 to S2
Figure S1. Locations of aircraft observations used in this study for (a) East Asia, (b) North America, and (c) Alaska/Arctic.

Table S1. Mean and standard deviation (std) of data–model mismatch between each flux inversion and aircraft-based CO$_2$ observations over East Asia, North America, and Alaska/Arctic. Posterior-simulated-CO$_2$ was calculated at $4^\circ \times 5^\circ$ spatial resolution.

| Region      | data set | prior NEE | East Asia | North America | Alaska/Arctic |
|-------------|----------|-----------|-----------|---------------|---------------|
|             |          | mean (ppm) | std (ppm) | mean (ppm) | std (ppm) | mean (ppm) | std (ppm) |
| prior       | SiB3     | -0.06     | 0.85      | 0.08         | 0.97         | -0.84      | 1.61       |
|             | CASA     | -0.01     | 0.76      | 0.26         | 0.56         | -0.59      | 1.36       |
|             | FLUXCOM  | 1.18      | 0.70      | 1.54         | 0.57         | 1.24       | 1.00       |
|             | Mean NEE | 0.37      | 0.57      | 0.63         | 0.54         | -0.06      | 1.16       |
| TCCON       | SiB3     | 0.16      | 0.46      | 0.33         | 0.43         | -0.10      | 0.86       |
|             | CASA     | 0.33      | 0.74      | 0.65         | 0.57         | -0.02      | 1.30       |
|             | FLUXCOM  | 0.42      | 0.45      | 0.42         | 0.45         | -0.02      | 1.18       |
|             | Mean NEE | 0.30      | 0.42      | 0.43         | 0.47         | -0.05      | 1.05       |
| surface-only| SiB3     | 0.01      | 0.44      | 0.34         | 0.35         | -0.06      | 0.80       |
|             | CASA     | 0.13      | 0.71      | 0.48         | 0.50         | -0.14      | 1.22       |
|             | FLUXCOM  | 0.22      | 0.60      | 0.46         | 0.33         | -0.01      | 0.88       |
|             | Mean NEE | 0.12      | 0.43      | 0.43         | 0.31         | -0.07      | 0.93       |
| GOSAT-only  | SiB3     | 0.25      | 0.41      | 0.49         | 0.37         | -0.06      | 0.76       |
|             | CASA     | 0.14      | 0.36      | 0.43         | 0.36         | -0.17      | 0.81       |
|             | FLUXCOM  | 0.23      | 0.44      | 0.50         | 0.33         | 0.03       | 0.89       |
|             | Mean NEE | 0.21      | 0.33      | 0.47         | 0.32         | -0.06      | 0.79       |
| GOSAT + surface | SiB3     | 0.18      | 0.35      | 0.34         | 0.31         | -0.7       | 0.75       |
|             | CASA     | 0.15      | 0.39      | 0.42         | 0.36         | -0.03      | 0.89       |
|             | FLUXCOM  | 0.16      | 0.38      | 0.39         | 0.32         | 0.00       | 0.93       |
|             | Mean NEE | 0.16      | 0.31      | 0.38         | 0.32         | -0.03      | 0.84       |
Figure S2. Number of hourly-mean aircraft measurements between 3–8 km altitude above sea level per month for (a) East Asia, (b) North America, and (c) Alaska/Arctic.
Figure S3. Same as Fig. 3 but at $2^\circ \times 2.5^\circ$ spatial resolution (except for TCCON). Comparison of monthly mean measured and simulated aircraft-based CO$_2$ for (a) East Asia, (b) North America, and (c) Alaska/Arctic. For each region, the mismatch for (left to right) prior, surface-only, GOSAT-only, and GOSAT+surface+TCCON simulated CO$_2$ are shown. The top panel shows a scatter plot of the simulated aircraft-based CO$_2$ against the measured aircraft-based CO$_2$, and the error bars indicate the spread in posterior NEE. The lower panel shows the mean data–model mismatch for each month, with error bars showing the range of monthly mean mismatched over the six-years and inversion set-ups. Colors correspond to the month of year.
Figure S4. Adjoint sensitivity of aircraft-based CO\textsubscript{2} measurements to surface fluxes for measurements over (a) East Asia, (b) North America, and (c) Alaska/Arctic. Black boxes show the location of aircraft-based CO\textsubscript{2} measurements.
Figure S5. Same as Fig. 8 but for Eurasia during (left-to-right) May, June, July and August of 2010. Monthly anomalies in (a) GOSAT $X_{CO_2}$ (ppm, $4^\circ \times 5^\circ$ grid cells) and surface site CO$_2$ (ppm divided by four, circles), (b) GOSAT-only posterior NEE, (c) surface-only posterior NEE, (d) GOSAT+surface posterior NEE, (e) MERRA-2 soil temperature anomalies (K), and (f) ESA CCI soil moisture.
Figure S6. Detrended zonal-monthly mean high-gain nadir GOSAT $X_{CO_2}$ retrieved by (a) ACOS 7.3 and (b) OCFP v7.1. (c) Difference in $X_{CO_2}$ between the two retrieval algorithms.

Figure S7. Data–model mismatch of the (a) ACOS 7.3 and (b) OCFP v7.1 GOSAT high-gain nadir $X_{CO_2}$ measurements as a function of latitude and time for the surface-only flux inversion.
Table S2. Mean and standard deviation (std) of data–model mismatch between each flux inversion and aircraft-based CO$_2$ observations over East Asia, North America, and Alaska/Arctic.

Posterior-simulated-CO$_2$ was calculated at $2^\circ \times 2.5^\circ$ spatial resolution.

| Region | data set | prior NEE | East Asia | North America | Alaska/Arctic |
|--------|----------|-----------|-----------|---------------|---------------|
|        |          | mean (ppm) | std (ppm) | mean (ppm) | std (ppm) | mean (ppm) | std (ppm) |
| 4prior | SiB3     | 0.57      | 0.94      | 0.56        | 1.03        | 0.01       | 1.56       |
|        | CASA     | -0.05     | 0.73      | 0.18        | 0.57        | -0.54      | 1.20       |
|        | FLUXCOM  | 1.16      | 0.75      | 1.39        | 0.62        | 1.19       | 0.90       |
|        | Mean NEE | 0.56      | 0.62      | 0.71        | 0.60        | 0.22       | 1.00       |
| surface-only | SiB3     | 0.01      | 0.44      | 0.26        | 0.40        | 0.03       | 0.73       |
|          | CASA     | 0.11      | 0.69      | 0.38        | 0.57        | -0.06      | 1.04       |
|          | FLUXCOM  | 0.22      | 0.62      | 0.35        | 0.39        | 0.06       | 0.79       |
|          | Mean NEE | 0.11      | 0.45      | 0.33        | 0.38        | 0.01       | 0.79       |
| GOSAT-only | SiB3     | 0.25      | 0.38      | 0.42        | 0.38        | 0.03       | 0.65       |
|          | CASA     | 0.18      | 0.39      | 0.37        | 0.39        | -0.07      | 0.72       |
|          | FLUXCOM  | 0.24      | 0.46      | 0.42        | 0.36        | 0.14       | 0.75       |
|          | Mean NEE | 0.22      | 0.35      | 0.40        | 0.35        | 0.03       | 0.68       |
| GOSAT | +surface | SiB3     | 0.20      | 0.37      | 0.28        | 0.33        | 0.06       | 0.66       |
|        | CASA     | 0.15      | 0.40      | 0.33        | 0.39        | 0.04       | 0.78       |
|        | FLUXCOM  | 0.22      | 0.38      | 0.36        | 0.32        | 0.15       | 0.78       |
|        | Mean NEE | 0.19      | 0.33      | 0.32        | 0.32        | 0.08       | 0.72       |