



Carbon Monitoring System Flux Net Biosphere Exchange 2020 (CMS-Flux NBE 2020)

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**Abstract**. Here we present a global and regionally-resolved terrestrial net biosphere exchange (NBE) dataset with corresponding uncertainties between 2010–2018: CMS-Flux NBE 2020. It is estimated using the NASA Carbon Monitoring System Flux (CMS-Flux) top-down flux inversion system that assimilates column CO<sub>2</sub> observations from Greenhouse gases Observing SATellite (GOSAT) and the NASA's Observing Carbon Observatory -2 (OCO-2). The regional

- SATellite (GOSAT) and the NASA's Observing Carbon Observatory -2 (OCO-2). The region monthly fluxes are readily accessible as tabular files, and the gridded fluxes are available in
- 32 NetCDF format. The fluxes and their uncertainty estimates are evaluated by extensively
- 33 comparing the posterior CO<sub>2</sub> mole fractions with aircraft CO<sub>2</sub> observations. We describe the
- 34 characteristics of the dataset as global total, regional climatological mean, and regional annual
- 35 fluxes and seasonal cycles. We find that the global total fluxes of the dataset agree with
- 36 atmospheric CO<sub>2</sub> growth observed by the surface-observation network within uncertainty.
- 37 Averaged between 2010 and 2018, the tropical regions range from close-to neutral in tropical
- 38 South America to a net source in Africa; these contrast with the extra-tropics, which are a net
- 39 sink of  $2.5 \pm 0.3$  gigaton carbon per year. The regional satellite-constrained NBE estimates
- 40 provide a unique perspective for understanding the terrestrial biosphere carbon dynamics and
- 41 monitoring changes in regional contributions to the changes of atmospheric CO<sub>2</sub> growth rate.
- 42 The gridded and regional aggregated dataset can be accessed at:
- 43 https://doi.org/10.25966/4v02-c391 (Liu et al., 2020).



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1 Introduction

New "top-down" inversion frameworks that harness satellite observations provide an important complement to global aggregated fluxes (e.g., Global Carbon Project, Friedlingstein et al., 2019) and inversions based on surface CO<sub>2</sub> observations (e.g., Crowell et al., 2019). These satelliteconstrained estimates resolve regional fluxes, and also disentangle net biosphere exchange (NBE) into constituent carbon fluxes including plant gross primary productivity (GPP) and biomass burning through solar-induced fluorescence and carbon monoxide proxies, respectively (Bowman et al., 2017, Liu et al., 2017). Both the spatial and process resolution are critical for evaluating models and reducing uncertainties about future carbon-climate feedbacks (e.g., Friedlingstein et al., 2014). The NBE are far more variable than ocean fluxes (Lovenduski and Bonan, 2017) or fossil fuel emissions (Yin et al, 2019), and are thus the focus of this dataset estimated from a topdown atmospheric CO<sub>2</sub> inversion of satellite column CO<sub>2</sub> dry-air mole fraction (X<sub>CO2</sub>). We present the global and regional NBE dataset as a series of maps, time series and tables, and disseminate it as a public dataset for further analysis and comparison to other sources of flux information. Finally, we provide a comprehensive evaluation of both mean and uncertainty estimates against an independent airborne dataset. Subsequent papers will present the partitioning of the NBE into constituent gross fluxes.

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Global top-down atmospheric CO<sub>2</sub> flux inversions have been historically used to estimate regional terrestrial NBE, which is a sum of net ecosystem exchange and biomass burning carbon fluxes. They make uses of the spatiotemporal variability of atmospheric CO<sub>2</sub>, which is dominated by NBE, to infer net carbon exchange at the surface (Chevallier et al., 2005; Baker et al., 2006; Liu et al., 2014). The accuracy of the NBE from top-down flux inversion is determined by the density and





69 accuracy of the CO<sub>2</sub> observations, the accuracy of modeled atmospheric transport, and knowledge

of the prior uncertainties of the flux inventories.

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For CO<sub>2</sub> flux inversions based on high precision *in situ* and flask observations, the measurement error is low (<0.2 parts per million (ppm)) and not a significant source of error; however, these observations are limited spatially, and are concentrating primarily over North America (NA) and

observations are limited spatially, and are concentrating primarily over North America (NA) and

Europe (Crowell et al., 2019). Satellite  $X_{CO2}$  from  $CO_2$ -dedicated satellites, such as the Greenhouse

Gases Observing Satellite (GOSAT) (launched in July 2009) and the Observing Carbon

Observatory 2 (OCO-2) (Crisp et al., 2017) have much broader spatial coverage (O'Dell et al.,

2018), and fill the observational gaps of conventional surface CO<sub>2</sub> observations, but they have up

to an order of magnitude higher single-sounding uncertainty and potential systematic errors

compared to the in situ and flask CO2 observations. Recent progress in instrument error

characterization, spectroscopy, and retrieval methods have significantly improved the accuracy

and precision of the X<sub>CO2</sub> retrievals (O'Dell et al., 2018; Kiel et al., 2019). The single sounding

random error of X<sub>CO2</sub> from OCO-2 is ~1.0 ppm (Kulawik et al., 2019). A recent study by Byrne et

al. (2020) shows less than a 0.5 ppm difference between posterior  $X_{CO2}$  constrained by a recent

data set, ACOS-GOSAT b7 X<sub>CO2</sub> retrievals, and those constrained by conventional surface CO<sub>2</sub>

observations. Chevallier et al. (2019) also showed that OCO-2 based flux inversion had similar

performance to surface CO<sub>2</sub> based flux inversions when comparing posterior CO<sub>2</sub> mole fractions

to aircraft CO2 in the free troposphere. Results from these studies show that systematic

uncertainties in CO2 retrievals from satellites are comparable to, or smaller than, other uncertainty

90 sources in atmospheric inversions (e.g. transport).





A newly-developed biogeochemical model-data fusion system, CARDAMOM, made progress in producing NBE uncertainties, along with mean values that are consistent with a variety of observations assimilated through a Markov Chain Monte Carlo (MCMC) method (Bloom et al., 2016; 2020). Transport model errors in general have also been reduced relative to earlier transport model intercomparison efforts, such as TRANSCOM 3 (Gurney et al., 2004; Gaubert et al., 2019). Advancements in satellite retrieval, transport, and prior terrestrial biosphere modeling have led to more mature inversions constrained by satellite  $X_{\rm CO2}$  observations.

Two satellites, GOSAT and OCO-2, have now produced more than 10 years of observations. Here we harness the CMS-Flux inversion framework (Liu et al., 2014; 2017; 2018; Bowman et al., 2017) to generate an NBE product: CMS-Flux NBE 2020, by assimilating both GOSAT and OCO-2 from 2010–2018. The dataset is the longest satellite-constrained NBE product so far. The CMS-Flux framework exploits globally available  $X_{\rm CO2}$  to infer spatially-resolved total surface-atmosphere exchange, which can be subsequently decomposed into individual fluxes using ancillary measurements (i.e., GPP, respiration, fires, fossil fuel, etc.). The flux estimates from the CMS-Flux framework have been used to assess the impacts of El Niño on terrestrial biosphere fluxes (Bowman et al, 2017; Liu et al, 2017) and the role of droughts in the North America (NA) carbon balance (Liu et al, 2018). These fluxes have furthermore been ingested into land-surface data assimilation systems to quantify heterotrophic respiration (Konings et al., 2019), evaluate structural and parametric uncertainty in carbon-climate models (Quetin et al., 2020), and inform climate dynamics (Bloom et al., 2020). We present the regional NBE and its uncertainty based on two types of regional masks: (1) latitude and continent; and )2) distribution of biome types (defined





by plant functional types), and continent. The gridded NBE dataset and its uncertainty are also

available, so that users can aggregate the fluxes and uncertainties based on self-defined regions.

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117 The outline of the paper is as follows: Section 2 describes methods, and Sections 3 and 4 describe

the dataset and the major NBE characteristics, respectively. We extensively evaluate the posterior

fluxes and uncertainties by comparing the posterior CO<sub>2</sub> mole fractions against aircraft

observations and a gross primary production (GPP) product (section 5). In Section 6, we discuss

the strength and weakness, and potential usage of the data. A summary is provided in Section 7,

and Section 8 is dataset availability and future plan.

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# 2 Methods

## 125 **2.1 CMS-Flux inversion system**

126 The CMS-Flux framework is summarized in Figure 1. The center of the system is the CMS-Flux

127 inversion system, which optimizes NBE and air-sea net carbon exchanges with a 4D-Var inversion

128 system (Liu et al., 2014). In the current system, we assume that no uncertainty in fossil fuel

emissions, since the uncertainty in fossil fuel emissions at regional scales is substantially less than

NBE uncertainties, which is a widely adopted assumption in global flux inversion systems (e.g.,

131 Crowell et al., 2019). The 4D-Var minimizes a cost function that include the sum of two terms:

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$$J(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + (\mathbf{y} - h(\mathbf{x}))^T \mathbf{R}^{-1} (\mathbf{y} - h(\mathbf{x})) \quad (1)$$

133 The first term measures the differences between the optimized fluxes and the prior fluxes

normalized by the prior flux error covariance **B**, and the second term measures the differences

between observations (y) and the corresponding model simulated value (h(x)) normalized by the

observation error covariance **R**. The term  $h(\cdot)$  is the observation operator that calculates



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observation-equivalent model-simulated  $X_{CO2}$ . The 4D-Var uses the adjoint (i.e., the backward integration of the transport model) (Henze et al., 2004) of the GEOS-Chem transport model to calculate the sensitivity of the observations to surface fluxes. The configurations of the inversion system are summarized in Table 1. We run both the forward and adjoint at  $4^{\circ}$  x  $5^{\circ}$  spatial resolution, and optimize monthly NBE and air-sea carbon fluxes at each grid point from January 2010 to December 2018. Inputs for the system include prior carbon fluxes, meteorological drivers, and the satellite  $X_{CO2}$  (Figure 1). Section 2.2 (Table 2) describes the prior flux and its uncertainties, and section 2.3 (Table 3) describes the observations and the corresponding uncertainties.

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#### 2.2 The prior CO<sub>2</sub> fluxes and uncertainties

Prior CO<sub>2</sub> fluxes include NBE, air-sea net carbon fluxes, and fossil fuel emissions (see Table 2).

The data sources for the prior fluxes are listed in Table 7. Methods to generate prior ocean carbon

fluxes and fossil fuel emissions are documented in Brix et al., (2015), Caroll et al. (2020), and Oda

et al. (2018). The focus of this dataset is optimized terrestrial biosphere fluxes, so we briefly

describe the prior terrestrial biosphere fluxes and its uncertainties.

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We construct the NBE prior using the CARDAMOM framework (Bloom et al., 2016).

CARDAMOM data assimilation system explicitly represents the time-resolved uncertainties in

NBE. The prior estimates are already constrained with multiple data streams accounting for

measurement uncertainties following a similar Bayesian approach used in the 4D-variational

approach. We use the CARDAMOM setup as described by Bloom et al. (2016, 2020) resolved at

monthly timescales; data constraints include GOME-2 solar-induced fluorescence (Joiner et al.,

2013), MODIS Leaf Area Index (LAI), and biomass and soil carbon (details on the data





160 assimilation are provided in Bloom et al. (2020)). In addition, mean GPP and fire carbon emissions 161 from 2010 - 2017 are constrained by FLUXCOM GPP (Tramontana et al., 2016) and GFEDv4.1s 162 (Randerson et al., 2018) respectively, both assimilated with an uncertainty of 20%. We use the 163 Olsen and Randerson (2001) approach to downscale monthly GPP and respiration fluxes to 3-164 hourly timescales, based on ERA-interim re-analysis of global radiation and surface temperature. 165 Fire fluxes are downscaled using the GFEDv4.1 daily and diurnal scale factors on monthly 166 emissions (Giglio et al., 2013). Posterior CARDAMOM NBE estimates are then summarized as 167 NBE mean and standard deviation values. 168 169 The NBE from CARDAMON shows net carbon uptake of 2.3 GtC/year over the tropics and close 170 to neutral in the extratropics (Figure S1). The year-to-year variability (i.e., interannual variability, 171 IAV) estimated from CARDAMOM from 2010 –2017 is generally less than 0.1 gC/m<sup>2</sup>/day outside 172 of the tropics (Figure S1). Because of the weak interannual variability estimated by CARDAMOM, 173 we use the same 2017 NBE prior for 2018. 174 175 CARDAMOM generates uncertainty along with the mean state. The relative uncertainty over the 176 tropics is generally larger than 100%, and the magnitude is between 50% and 100% over the extra-177 tropics (Figure S2). We assume no correlation in prior flux errors in either space or time. Temporal 178 and spatial error correlation estimates can in principle be computed by CARDAMOM. We 179 anticipate incorporating these error correlations in subsequent versions of this dataset. 180 181 2.3 Column CO<sub>2</sub> observations from GOSAT and OCO-2 182 We use satellite-column CO2 retrievals from Atmospheric Carbon Observations from Space 183 (ACOS) team for both GOSAT (version 7.3) and OCO-2 (version 9) (Table 3). The use of the





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same retrieval algorithm and validation strategy adopted by ACOS team to process both GOSAT and OCO-2 spectra maximize the consistency between these two datasets. Both GOSAT and OCO-2 satellites carry high-resolution spectrometers optimized to return high precision measurements of reflected sunlight within CO<sub>2</sub> and O<sub>2</sub> absorption bands in the shortwave infrared (Crisp et al., 2012). Both satellites fly in a sun-synchronous orbit. GOSAT has a 13:00  $\pm$  0.15 hours local crossing time and a three-day ground track repeat cycle. The footprint of GOSAT is ~10.5 km in diameter in sun-nadir view (Crisp et al., 2012). The daily number of soundings processed by the ACOS-GOSAT retrieval algorithm is between a few hundreds to ~2000. Further quality control and filtering reduce the ACOS-GOSAT X<sub>CO2</sub> retrievals to 100 – 300 daily (Figure S5 in Liu et al., 2017). We only assimilate ACOS-GOSAT land nadir good quality observations. OCO-2 has a 13:30 local crossing time and 16-day ground track repeat cycle. The nominal footprints of OCO-2 are 1.25 km wide and ~2.4 km along the orbit. Because of its small footprint and sampling strategy, OCO-2 has many more X<sub>CO2</sub> retrievals than ACOS-GOSAT. OCO-2 has four observing modes: land nadir, land glint, ocean glint, and target. Following Liu et al. (2017), we only use land nadir observations from OCO-2 to generate a set of super observations by aggregating the observations within  $\sim$ 100 km (along the same orbit). The super observations have more uniform spatial coverage and are more comparable to the spatial representation of ACOS-GOSAT observations (see Figure S5 in Liu et al., 2017). We directly use observational uncertainty provided with ACOS-GOSAT b7.3 to represent the observation error, R, in Eq 1. The uncertainty of the OCO-2 super observations is the sum of the variability of  $X_{CO2}$  used to generate each individual super observation and the mean uncertainty





provided in the original OCO-2 retrievals. More detailed information about OCO-2 super observations can be found in Liu et al. (2017). Kulawik et al. (2019) showed that both OCO-2 and ACOS-GOSAT bias-corrected retrievals have mean biases of -0.1 ppm when compared against X<sub>CO2</sub> from Total Carbon Column Observing Network (TCCON) (Wunch et al., 2011), indicating consistency between ACOS-GOSAT and OCO-2 retrievals. The magnitude of observation errors used in **R** is generally above 1.0 ppm, larger than the sum of random error and biases in the observations. The ACOS-GOSAT b7.3 observations from July 2009–June 2015 are used to optimize fluxes between 2010 and 2014, and the OCO-2 X<sub>CO2</sub> observations from Sep 2014–June 2019 are used to optimize fluxes between 2015 and 2018.

The observational coverage of ACOS-GOSAT and OCO-2 is spatiotemporally dependent, with more coverage during summer than winter over the NH, and more observations over mid-latitudes than over the tropics (Figure S3). The variability (i.e., standard deviation) of annual total number of observations from 2010–2014 is within 4% of the annual mean number for ACOS-GOSAT. Except for a data gap in 2017 caused by a malfunction of OCO-2 instrument, the variability of annual total number of observations between 2015 and 2018 is within 8% of the annual mean number for OCO-2.

## 2.4 Uncertainty quantification

The posterior flux error covariance is analytically the inverse Hessian, which incorporates the transport, measurement, and background errors at the 4D-Var solution (Eq. 13 in Bowman et al, 2017). For large-order systems, the posterior errors cannot be explicitly calculated. Consequently, we rely on a Monte Carlo approach to quantify posterior flux uncertainties following Chevallier et al. (2010) and Liu et al. (2014). In this approach, an ensemble of flux inversions is carried out with





231 an ensemble of priors and simulated observations to sample the uncertainties of prior fluxes (i.e., 232 **B** in eq. 1) and observations (**R** in Eq. 1), respectively. The magnitude of posterior flux 233 uncertainties is a function of assumed uncertainties in prior fluxes and observations, as well as the density of observations. Since the density of GOSAT and OCO-2 observations are stable (section 234 235 2.3) within their respective data record, we characterize the posterior flux uncertainties for 2010 236 and 2015 only, and assume the flux uncertainties for 2011-2014 are the same as 2010 and flux 237 uncertainties for 2016–2018 are the same as 2015. 238 2.5 Evaluation of posterior fluxes 239 Direct NBE estimates from flux towers only provide a spatial representation of a few kilometers 240 (Running et al., 1999), not appropriate to evaluate regional NBE from top-down flux inversions. 241 Thus, we use two methods to indirectly evaluate the posterior NBE and its uncertainties. One is to compare annual NBE anomalies and seasonal cycle to a gross primary production (GPP) product. 242 243 The other is to compare posterior CO<sub>2</sub> mole fractions to independent aircraft observations (i.e., not 244 assimilated in the inversion). The second method has been broadly used to indirectly evaluate posterior fluxes from top-down flux inversions (e.g., Stephens et al., 2007; Liu and Bowman, 2016; 245 246 Chevallier et al., 2019; Crowell et al., 2019). 247 2.5.1 Evaluation against independent gross primary production (GPP) product 248 NBE is a small residual difference between two large terms: total ecosystem respiration (TER) 249 and GPP, plus fire. A positive NBE anomaly (i.e., less uptake from the atmosphere) has been 250 shown to correspond to reduced GPP caused by climate anomalies (e.g., Bastos et al., 2018), and the magnitude of net uptake is proportional to GPP in most biomes observed by flux tower 251 252 observations (e.g., Falk et al., 2008). Since NBE is related not only to GPP, the comparison to GPP 253 only serves as a qualitative measure of the NBE quality. For example, we would expect that the





posterior NBE seasonality to be anti-correlated with GPP in the temperate and high latitudes. In this study, we use FLUXSAT GPP (Joiner et al., 2018), which is an upscaled GPP product based on flux tower GPP observations and satellite-based geometry adjusted reflectance from the MODerate-resolution Imaging Spectroradiometer (MODIS) and solar-induced chlorophyll fluorescence observations from Global Ozone Monitoring Experiment – 2 (GOME-2) (Joiner et al., 2013). Joiner et al. (2018) show that the agreement between FLUXSAT-GPP and GPP from flux towers is better than other available upscaled GPP products.

### 2.5.2 Evaluation against aircraft CO<sub>2</sub> observations

The aircraft observations used in this study include those published in ObsPack August 2019 (CarbonTracker team, 2019), which include regular vertical profiles from flask samples collected on light aircraft by NOAA (Sweeney et al., 2015) and other laboratories, aircraft campaigns from Atmospheric Tomography (ATom, Wofsy et al., 2018) and HIAPER Pole-to-Pole (HIPPO, Wofsy et al., 2011), regular (two to four weekly) vertical profiles from the Instituto de Pesquisas Espaciais (INPE) over tropical South America (SA) (Gatti et al., 2014), and the O<sub>2</sub>/N<sub>2</sub> Ratio and CO<sub>2</sub> airborne Southern Ocean (ORCAS) Study aircraft campaign (Stephens et al., 2017) (Table 3). Figure 2 shows the aircraft observation coverage and density between 2010 and 2018. Most of the aircraft observations are concentrated over NA. ATom had four (1–4) campaigns between August 2016 to May 2018, spanning four seasons over the Pacific and Atlantic Ocean. HIPPO had five (1–5) campaigns over Pacific, and only HIPPO 3–5 occurred between 2010 and 2011. HIPPO 1–2 occurred in 2009. Based on the spatial distribution of aircraft observations, we divide the comparison into nine regions: Alaska, mid-latitude NA, Europe, East Asia, South Asia, Africa, Australia, Southern Ocean, and South America (Table 4 and Figure 2).





- We calculate several quantities to evaluate the posterior fluxes and its uncertainty with aircraft
- 278 observations. One is the monthly mean differences between posterior and aircraft CO<sub>2</sub> mole
- fractions. The second is the monthly root mean square errors (RMSE) over each nine sub-regions,
- which is defined as:

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$$RMSE = \left(\frac{1}{n} \sum_{i=1}^{n} (y_{aircraft}^{o} - y_{aircraft}^{b})_{i}^{2}\right)^{\frac{1}{2}}$$
 (2)

- where  $y_{aircraft}^{o}$  is  $i^{th}$  aircraft observation,  $y_{aircraft}^{b}$  is the corresponding posterior CO<sub>2</sub> mole
- fractions sampled at  $i^{th}$  aircraft locations, and n is the number of aircraft observations over each
- region. The RMSE is computed over the *n* aircraft observations within one of the nine sub-regions.
- 285 The mean differences indicate the magnitude of mean posterior CO<sub>2</sub> bias, while the RMSE
- 286 includes both random and systematic errors in posterior CO<sub>2</sub>. The bias and RMSE could be due to
- errors in either posterior fluxes or transport or both. When transport errors are smaller than errors
- 288 in posterior fluxes, the magnitude of biases and *RMSE* indicates the accuracy of posterior fluxes.
- 290 To evaluate the magnitude of posterior flux uncertainty estimates, we compare RMSE against the
- 291 standard deviation of ensemble simulated aircraft observations (equation 3) from the Monte Carlo
- method ( $RMSE_{MC}$ ). The quantity  $RMSE_{MC}$  can be written as:

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$$RMSE_{MC} = \left[\frac{1}{nens} \sum_{iens=1}^{nens} ((y_{aircraft}^{b(MC)})_{iens} - \bar{y}_{aircraft}^{b(MC)})^2\right]^{\frac{1}{2}} (3)$$

- The variable  $(y_{aircraft}^{b(MC)})_{iens}$  is the  $i^{th}$  ensemble member of simulated aircraft observations from
- Monte Carlo ensemble simulations,  $\bar{y}_{aircraft}^{b(MC)}$  is the mean, and *nens* is the total number of ensemble
- 296 members. For simplicity, in equation (3), we drop the indices for the aircraft observations used in
- 297 equation (2). In the absence of transport errors, when the estimated posterior flux uncertainty
- reflects the "true" posterior flux uncertainty, we show in the Appendix that:





- $299 RMSE^2 = R_{aircraft} + RMSE_{MC}^2 (4)$
- 300 where  $R_{aircraft}$  is the aircraft observation error variance, which could be neglected on regional
- 301 scales. We further calculate the ratio r between RMSE and RMSE<sub>MC</sub>:

$$302 r = \frac{RMSE}{RMSE_{MC}} (5)$$

- 303 A ratio close to one indicates that the posterior flux uncertainty reflects the true uncertainty in the
- 304 posterior fluxes when the transport errors are small.
- 306 The presence of transport errors will make the comparison between RMSE and RMSE<sub>MC</sub>
- 307 potentially difficult to interpret. Even when  $RMSE_{MC}$  represents the actual uncertainty in posterior
- 308 fluxes, the RMSE could be larger than  $RMSE_{MC}$ , since the differences between aircraft
- 309 observations and model simulated posterior mole fractions RMSE could be due to errors in both
- 310 transport and the posterior fluxes, while  $RMSE_{MC}$  only reflects the impact of posterior flux
- 311 uncertainty on simulated aircraft observations. In this study, we assume the primary sources of
- 312 *RMSE* come from errors in posterior fluxes.
- 314 The RMSE and RMSE<sub>MC</sub> comparison only shows differences in  $CO_2$  space. We further calculate
- 315 the sensitivity of RMSE to posterior flux using GEOS-Chem adjoint. We first define a cost
- 316 function J as:
- 317  $I = RMSE^2$  (6)
- The sensitivity of the mean-square error to a flux, x, at location i and month j is

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$$w_{i,j} = \frac{\partial J}{\partial x_{i,j}} \times x_{i,j}$$
 (7)





- 320 This sensitivity is normalized by the flux magnitude. Equation 7 can be interpreted as the
- sensitivity of the  $RMSE^2$  to a fractional change in the fluxes. We can estimate the time-integrated
- magnitude of the sensitivity over the entire assimilation window by calculating:

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$$S_i = \frac{\sum_{j=1}^{M} |w_{i,j}|}{\sum_{k=1}^{P} \sum_{j=1}^{M} |w_{k,j}|}$$
 (8)

- 324 where P is the total number of grid points and M is the total number of months from the time of
- 325 the aircraft data to the beginning of the inversion. The numerator of equation (8) quantifies the
- 326 absolute total sensitivity of the  $RMSE^2$  to the fluxes at the  $i^{th}$  grid. Normalized by the total absolute
- sensitivity across the globe, the quantity  $S_i$  indicates the relative sensitivity of  $RMSE^2$  to fluxes at
- 328 the  $i^{th}$  grid point. Note that  $S_i$  is unitless, and it only quantifies sensitivity, not the contribution of
- fluxes at each grid to  $RMSE^2$ .

## 2.6 Regional masks

3 Dataset description

- We provide posterior NBE from 2010 2018 using two sets of aggregated regions, for a few
- 333 selected FLUXNET tower sites, and the underlying gridded product. The regional mask in Figure
- 334 3A is based on a combination of seven plant function types condensed from MODIS IGBP and the
- 335 TRANSCOM -3 region mask (Gurney et al., 2004). There are 28 regions in Figure 3A: six in NA,
- four in SA, five in Eurasia (north of 40°N), three in tropical Asia, three in Australia, and seven in
- Africa. The regional mask in Figure 3B is based on latitude and continents, and there are 13 regions
- 338 in total.

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We present the gridded fluxes as globally, latitudinally, and regionally time series. We show the

343 nine-year average fluxes aggregated into 28 and 13 geographic regions (Figure 3). The





aggregations are geographic (latitude and continent), bio-climatic (biome by continent), and flux-oriented (for a set of selected flux sites). For each region in the geographic and biome aggregations, we show nine-year mean annual net fluxes and uncertainties, and then the annual fluxes for each region as a set of time-series plots. The month-by-month fluxes and uncertainties are available in tabular format, so the actual aggregated fluxes may be readily compared to bottom-up extrapolated fluxes and Earth System models. Users can also aggregate the gridded fluxes and uncertainties based on their own defined regional masks. Table 5 provides a complete list of all data products available in the dataset. In section 4, we describe the major characteristics of the dataset.

#### 4 Characteristics of the dataset

#### 4.1 Global fluxes

The annual atmospheric  $CO_2$  growth rate, which is the sum of fossil fuel emissions and total annual sink over land and ocean, is well-observed by NOAA surface  $CO_2$  observing network (https://www.esrl.noaa.gov/gmd/ccgg/ggrn.php) (Freidlingstein et al., 2019). We compare the global total flux estimates constrained by GOSAT and OCO-2 with the NOAA  $CO_2$  growth rate from 2010–2018, and discuss the mean carbon sink over land and ocean. Over these nine years, the satellite-constrained atmospheric  $CO_2$  growth rate agrees with the NOAA observed  $CO_2$  growth rate within the uncertainty of posterior fluxes (Figure 4). The mean annual global surface  $CO_2$  flux (in Gt C/yr) is derived from the NOAA observed  $CO_2$  growth rate (in ppm/yr) using a conversion factor of 2.124 GtC/ppm (Le Quéré et al., 2018). The estimated growth rate has the largest discrepancy with the NOAA observed growth rate in 2014, which may be due to a failure of one of the two solar paddles in May 2014 (Kuze et al., 2016). Over the nine years, the estimated total accumulated carbon in the atmosphere is  $41.5 \pm 2.4$  GtC, which is slightly lower than the accumulated carbon based on NOAA  $CO_2$  growth rate ( $45.2 \pm 0.4$  GtC). On average, the land sink is  $20 \pm 8\%$  of fossil



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fuel emissions, and the ocean sink is  $30 \pm 1\%$  of fossil fuel emissions (Figure 4). These numbers are within the ranges of the corresponding estimates from GCP 2019 (Freidlingstein et al., 2019). The mean NBE and ocean sink from GCP 2019 are  $21 \pm 10\%$  (~1.0 GtC estimated residual NBE uncertainty) and  $26 \pm 5\%$  (~0.5 GtC estimated ocean flux uncertainty) of fossil fuel emissions respectively between 2010-2018. The GCP NBE here is calculate as the residual differences between fossil fuel, ocean fluxes, and atmospheric CO2 growth rate, and it is also equivalent to the sum of carbon fluxes from land use changes, land sink, and residual balance reported by GCP. Over these nine years, we estimate that the land sink ranges from 37% of fossil fuel emissions in 2011 (a La Niña year) to only 5% in 2015 (an El Niño year), consistent with GCP estimated range of 35% in 2011 to 7% in 2015. We estimate that the ocean sinks range from 39% in 2015 to 23% of fossil fuel emissions in 2012, larger than the GCP estimated ocean flux ranges of 25% to 28% of fossil fuel emissions (Freidlingstein et al., 2019). 4.2 Mean regional fluxes and uncertainties Figure 5 shows the nine-year mean regional annual fluxes, uncertainty, and its variability between 2010-2018. Table 6 shows an example of the dataset corresponding to Figure 5 A, C, and E. It shows large net carbon uptake occurs over Eurasia, NA, and Southern Hemisphere (SH) midlatitudes. The largest net carbon uptake is over eastern US (-0.4  $\pm$  0.1 GtC (1 $\sigma$  uncertainty)) and high latitude Eurasia (-0.4  $\pm$  0.1 GtC) (Figure 5A, B). We estimate a net land carbon sink of 2.5  $\pm$ 0.3 GtC/year between 2010–2013 over the NH mid to high latitudes, which agrees with  $2.4 \pm 0.6$ GtC estimates over the same time periods based on a two-box model (Ciais et al., 2019). Net uptake in the tropics ranges from close-to-neutral in tropical South America ( $0.0 \pm 0.1$  GtC) to a net source in northern Africa ( $0.6 \pm 0.2$  GtC) (Figure 5A, B). The tropics exhibit both large uncertainty and

large variability. The NBE interannual variability over northern Africa and tropical SA are 0.5 GtC





and 0.3 GtC respectively, larger than the 0.2 GtC and 0.1 GtC uncertainty (Figure 5C, D). We also find collocation of regions with large NBE and GPP interannual variability (Figure S4).

#### 4.3 Interannual variabilities and uncertainties

Here we present hemispheric and regional NBE interannual variabilities and corresponding uncertainties (Figures 6 and 7, and corresponding tabular data files). In Figure 6, we further divide the globe into three large latitude bands: tropics (20°S–20°N), NH extra-tropics (20°N–85°N), and SH extra-tropics (60°S–20°S). The tropical NBE contributes 90% to the global NBE interannual variability (IAV). The IAV of NBE over the extra-tropics is only about one-third of that over the tropics. The dominant role of tropical NBE in the global IAV of NBE agrees with Figure 4 in Sellers et al. (2018). The top-down global annual NBE anomaly is within the 1.0 GtC/yr uncertainty of residual NBE (i.e., fossil fuel – atmospheric growth – ocean sink) calculated from GCP-2019 (Friedlinston et al., 2019) (Figure 6).

Figure 7 shows the annual NBE anomalies and uncertainties over a few selected regions. Positive NBE indicates reduced net uptake relative to the 2010–2018 mean, and vice versa. Also shown in Figure 7 are GPP anomalies estimated from FLUXSAT. Positive GPP indicates increased productivity, and vice versa. GPP drives NBE in years where anomalies are inversely correlated (e.g., positive NBE and negative GPP), and TER drives NBE in years where anomalies of GPP and NBE have the same sign or weakly correlated. Over tropical SA evergreen broadleaf forest, the largest positive NBE anomalies occur during 2015–2016 El Niño, corresponding to large reductions in productively, consistent with Liu et al. (2017). In 2017, the region sees increased net uptake and increased productivity, implying a recovery from the 2015–2016 El Niño event. The





variability in GPP explains 80% of NBE variability over this region over the nine-year period. In Australian shrubland, our inversion captures the increased net uptake in 2010 and 2011 due to increased precipitation (Pouter et al., 2014) and increased productivity. The variability in GPP explains 70% of the interannual variability in NBE. Over tropical south America Savanna, the NBE interannual variability also shows strong negative correlations with GPP, with GPP explaining 40% of NBE interannual variability. Over the mid-latitude regions where the IAV is small, the R<sup>2</sup> between GPP and NBE is also small (0.0–0.5) as expected. But the increased net uptake generally corresponds to increased productivity. We also do not expect perfect negative correlation between NBE anomalies and GPP anomalies, as discussed in section 2.5. The comparison between NBE and GPP provides insight into when and where net fluxes are likely dominated by productivity.

#### 4.4 Seasonal cycle

We provide a top-down  $CO_2$  constrained regional mean NBE seasonal cycle and its variability and uncertainty. The seasonal cycle of NBE, including its phase (i.e., transition from source to sink) and amplitude (peak-to-trough difference), have large uncertainties, not only over the less-observed tropical regions, but also over the extra-tropics (e.g., Yang et al., 2007; Keppel-Aleks et al., 2012). Figure 8 shows NBE and GPP seasonal cycles for six selected regions. In general, the months that have larger productivity corresponds to months with a net uptake of carbon from the atmosphere. The NH mid-to-high latitudes have larger seasonal cycle amplitudes (Figure 8A, B) compared to the other regions, and their NBE seasonalities are more closely linked to that of GPP ( $R^2 = 0.9$ ). In the tropics, the relationship between NBE and GPP seasonality is less clear partially



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437 5 Evaluation against independent aircraft CO<sub>2</sub> observations 438 5.1 Comparison to aircraft observations over nine sub-regions 439 In this section, we evaluate posterior CO<sub>2</sub> against aircraft observations over nine sub-regions listed 440 in Table 4 and Figure 2. We compare the posterior to aircraft CO<sub>2</sub> mole fractions above planetary 441 boundary layer and up to mid troposphere (1-5 km) at the locations and time of aircraft 442 observations, and then calculate the monthly mean error statistics between 1-5 km. The aircraft 443 observations between 1-5 km are more sensitive to regional fluxes (Liu et al., 2015; Liu and 444 Bowman, 2016). Scatter plots in the left column of Figure 9 show regional monthly mean de-445 trended aircraft CO<sub>2</sub> observations (x-axis) versus the simulated detrended posterior CO<sub>2</sub> (y-axis). 446 We used NOAA global CO<sub>2</sub> trend to detrend both the observations and model simulated mole 447 fractions (ftp://aftp.cmdl.noaa.gov/products/trends/co2/co2 trend gl.txt). Over the NH regions (A. 448 B, C, D) and Africa (F), the R<sup>2</sup> is equal or above 0.9, which indicates that the posterior CO<sub>2</sub> captures 449 the observed seasonality. The low R<sup>2</sup> (0.7) value in South Asia is caused by one outlier. Over

due to the weak seasonality of NBE (Figure 8E, F). The variability and uncertainty of monthly

mean fluxes are larger over the tropics and the SH extratropics than over the NH extratropics.

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seasonality over these regions.

The right panel of Figure 9 shows the monthly mean differences between posterior  $CO_2$  and aircraft observations (black), the number of aircraft observations (blue bar, right y-axis), *RMSE* (equation 2) (blue line), and *RMSE<sub>MC</sub>* (equation 3) (red line). The magnitude of mean differences between posterior  $CO_2$  and aircraft observations is less than 0.5 ppm except over Southern Ocean, which has a -0.8 ppm bias. The mean differences between posterior  $CO_2$  and aircraft observations are

Southern Ocean, Australia, and SA, the R<sup>2</sup> is between 0.2 and 0.4, reflecting weaker CO<sub>2</sub>



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458 primarily caused by errors in transport and biases in assimilated satellite observations, while 459  $RMSE_{MC}$  is 'internal flux error' projected into mole fraction space. With the exception of the 460 Southern Ocean, for all regions mean bias is significantly less than  $RMSE_{MC}$ , which suggests that transport and data bias in satellite observations may be much smaller than the internal flux errors. 462 463 As demonstrated in section 2.5, comparing RMSE and  $RMSE_{MC}$  is a test of the accuracy of posterior 464 flux uncertainty estimate. Over all the regions, the differences between RMSE and RMSE<sub>MC</sub> are 465 smaller than 0.3 ppm, which indicates a comparable magnitude between empirical posterior flux 466 uncertainty estimates from Monte Carlo method and the actual posterior flux uncertainty over the 467 regions that these aircraft observations are sensitive to. These aircraft observations are sensitive to 468 fluxes over a broad region as shown in Figure S5. 469 470 5.2 Comparison to aircraft observations from ATom and HIPPO aircraft campaigns Figures 10 and 11 show comparisons to aircraft CO<sub>2</sub> from ATom 1-4 campaigns spanning four 472 seasons, and HIPPO 3-5 over the Pacific Ocean between 1-5 km. The vertical curtain comparisons 473 are shown in Figure S6 and S7. The mean differences between posterior CO<sub>2</sub> and aircraft CO<sub>2</sub> are 474 quite uniform (within 0.5 ppm) throughout the column except over the Atlantic Ocean during 475 ATom 1–2 and the Southern Ocean during ATom 1 (Figures S6 and S7). Also shown in Figures 476 10 and 11 are RMSE of each aircraft campaign (middle column) and the ratio between RMSE and 477  $RMSE_{MC}$  (right column). A ratio larger than one between RMSE and  $RMSE_{MC}$  indicates errors in

either transport or low of posterior flux uncertainty estimates (section 2.5).



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Over most of flight tracks during ATom 1-4, the posterior CO<sub>2</sub> errors are between -0.5 and 0.5 ppm, the RMSE is smaller than 0.5 ppm, and the ratio between RMSE and RMSE<sub>MC</sub> is smaller than or equal to 1. However, off the coast of Africa during ATOM -1 and -2 and over Southern Ocean during ATOM-1, the mean differences between posterior CO2 and aircraft observations are larger than 0.5 ppm. During ATOM-1 (29 July – 23 Aug 2016), the mean differences between posterior CO<sub>2</sub> and aircraft CO<sub>2</sub> show large negative biases, while during ATOM-2 (26 Jan 2017–21 Feb 2017), it has large positive biases off the coast of Africa. The ratio between RMSE and RMSE<sub>MC</sub> is significantly larger than one over these regions, which indicates an underestimation of posterior flux uncertainty or large magnitude of transport errors during that time period. We further run adjoint sensitivity analyses over the three regions with ratios significantly larger than one to identify the posterior fluxes that could contribute to the large differences between posterior CO<sub>2</sub> and aircraft observations during ATOM 1-2. We run the adjoint model backward for three months from the observation time and calculate  $S_i$  defined in equation (7). Adjoint sensitivity analysis indicates that the large mismatch between aircraft observations and model simulations during ATOM-1 and -2 off the coast of Africa could be potentially driven by errors in posterior fluxes over tropical Africa (Figure S8). These large posterior CO<sub>2</sub> errors and large ratio over Southern Ocean during ATOM-1 are driven by flux errors in oceanic fluxes around 30°S and over Australia (Figure S9). During the HIPPO aircraft campaigns, the absolute errors in posterior CO<sub>2</sub> across Pacific are less than 0.5 ppm except over the Arctic Ocean and over Alaska in summer (Figure 11), consistent with Figure 10A. The large errors over the Arctic Ocean may be related to both transport errors



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and the accuracy of high latitude fluxes. Byrne et al. (2020) provide a brief summary of these challenges in simulating CO2 over high latitudes with 4° x 5° resolution transport model. Increasing the resolution of the transport model may reduce transport errors over high latitudes. We run adjoint sensitivity analysis over the high-latitude regions where the differences between posterior CO<sub>2</sub> and aircraft observations are large (Figure 11). The adjoint sensitivity analysis (Figure S10) shows that the large errors over these regions could be driven by errors in fluxes over Alaska as well as broad NH mid-latitude regions. 6 Discussion Evaluation of posterior flux uncertainty estimates by comparing posterior CO<sub>2</sub> error statistics (RMSE, Equation 2) with the standard deviation of ensemble simulated CO<sub>2</sub> from Monte Carlo uncertainty quantification method (RMSE<sub>MC</sub>, equation 3) has its limitations. When RMSE and RMSE<sub>MC</sub> are similar in magnitude, this indicates small magnitude of transport errors and reasonable posterior uncertainty estimates. A much larger RMSE than RMSE<sub>MC</sub> could be due to errors in either transport or underestimation of posterior flux uncertainty or both. The presence of transport errors makes the interpretation of the RMSE and RMSE<sub>MC</sub> complex. A better, independent quantification of transport errors is needed in the future in order to rigorously use the comparison statistics between aircraft observations and posterior CO<sub>2</sub> to diagnose flux errors. Comparison to aircraft observations shows regionally-dependent accuracy in posterior fluxes. ATom observations show seasonally-dependent biases over the Atlantic, implying possible seasonally dependent errors in posterior fluxes over northern to central Africa. Therefore, we

recommend combining NBE with other ancillary variables, e.g., GPP, to better understand carbon





527 dynamics. Combining NBE with component carbon fluxes can shed light on the processes 528 controlling the changes of NBE (e.g., Bowman et al., 2017; Liu et al., 2017). NBE can be written 529 as: NBE = TER + fire - GPP (8) 530 where TER is total ecosystem respiration (TER) (Figure 1). Satellite carbon monoxide (CO) 531 532 observations provide constraints on fire emissions (Arellano et al, 2006, van der Werf, 2008; Jones 533 et al., 2009; Jiang et al., 2015, Bowman et al., 2017; Liu et al., 2017). In addition to FLUXSAT-534 GPP product used here, solar induced chlorophyll fluorescence (SIF) can be directly used as a 535 proxy for GPP (e.g., Parazoo et al, 2014). Once NBE, fire, and GPP carbon fluxes are quantified, 536 TER can be calculated as a residual (e.g., Bowman et al, 2017; Liu et al., 2017, 2018). 537 538 Because of the diffusive manner of atmospheric transport and the limited observation coverage, 539 the gridded flux values are not independent from each other. The errors and relative uncertainties 540 of the fluxes at each individual grid point are larger than regional aggregated fluxes. For the same 541 reason, comparing NBE with flux tower observations needs caution, though we provide NBE at a 542 few flux tower sites. 543 544 The variability and changes are more robust than the mean NBE fluxes from top-down flux 545 inversions in general (Baker et al., 2006b). The errors in transport and potential biases in 546 observations are mostly stable in time, so biases in the mean fluxes tend to cancel out when computing interannual variability and year-to-year changes (Schuh et al., 2019; Crowell et al., 547 548 2019).





The global fossil fuel emissions have  $\sim$ 5% uncertainty (GCP, 2019). However, they are regionally inhomogeneous. We neglect the uncertainties in fossil fuel emissions, which will introduce additional error in regions of rapid fossil fuel growth or in areas with noisier statistics (Yin et al., 2019). In the future, we will account for uncertainties in fossil fuel emissions.

The posterior NBE includes all types of land fluxes except fossil fuel emissions, which is equivalent to the sum of land use change fluxes and land sinks published by GCP. The sum of regional NBE and fossil fuel emissions is an index of the contribution of any specific region to the changes of atmospheric CO<sub>2</sub> growth rate. Even over the continental US, where fossil fuel emissions are ~1.5 GtC/year, the changes of regional NBE can significantly modify contributions to the changes of atmospheric CO<sub>2</sub> (Liu et al., 2018). Since NBE has high variability and its predicted changes in the future are likely to have large uncertainties, quantifying regional NBE is critical to monitoring regional contributions to atmospheric CO<sub>2</sub> growth rate, and ultimately to guide mitigation to limit warming to 1.5°C above pre-industrial level (IPCC, AR6).

## 7 Summary

Terrestrial biosphere carbon fluxes are the largest contributor to the interannual variability of the atmospheric CO<sub>2</sub> growth rate. Therefore, monitoring its change at regional scales is essential for understanding how it responds to CO<sub>2</sub>, climate and land use. Here, we present the longest terrestrial flux estimates and their uncertainties constrained by X<sub>CO2</sub> from 2010–2018 on self-consistent global and regional scales (CMS-Flux NBE 2020). We qualitatively evaluate the net flux estimates by comparing its variability with GPP variability, and provide comprehensive evaluation of posterior fluxes and the uncertainties by comparing posterior CO<sub>2</sub> with independent aircraft CO<sub>2</sub>.





The estimated posterior flux uncertainty agrees with the expected uncertainty in the posterior fluxes based on the comparison to aircraft CO<sub>2</sub> observations. This dataset can be used in understanding controls on regional NBE interannual variability, evaluating biogeochemical models, and provide support the monitoring of the regional contributions to the changes in atmospheric CO<sub>2</sub>.

#### 8 Data availability and future update

The CMS-Flux NBE 2020 data is available at: https://doi.org/10.25966/4v02-c391 (Liu et al., 2020). The regional aggregated fluxes are provided as *csv* files with file size ~10MB, and the gridded data is provided in NetCDF format with file size ~10MB. The full ensemble posterior fluxes used to estimate posterior flux uncertainties are provided in NetCDF format with file size ~20MB. Table 7 lists the sources of the data used in producing and evaluating the CMS-Flux NBE 2020 data product.

The quality of X<sub>CO2</sub> from satellite observations is continually improving. The OCO-2 v10 X<sub>CO2</sub> will be released in June 2020, and the full GOSAT record (June 2009–Jan 2020) processed by the same retrieval algorithm as OCO-2 will be released around the same time. Continuing to improving the quality of satellite observations and extending the NBE estimates beyond 2018 in the future will help us better understand interactions between terrestrial biosphere carbon cycle and climate and provide support in monitoring the regional contributions to the changes of atmospheric CO<sub>2</sub>. Thus, we plan a future update of the dataset on an annual basis, with a goal to support current scientific research and policy making.

## 9 Author contributions





JL designed the study and led the writing of the paper in close collaboration with KB and DS. LB helped generate the plots and created all the data files. AAB provided the prior of the terrestrial biosphere carbon fluxes. NP helped interpret the GPP evaluation. DM and DC generated the prior ocean carbon fluxes. TO generated the ODIAC fossil fuel emissions. JJ provided the FLUXSAT GPP product. BD and SW provided and contributed to the interpretation of HIPPO aircraft CO<sub>2</sub> observation comparisons. BS, KM, and CS provided ORCAS aircraft CO<sub>2</sub> observations and contributed interpretation of aircraft CO<sub>2</sub> observation comparisons. LVG and JM provided INPE aircraft CO<sub>2</sub> observations and contributed interpretation of aircraft CO<sub>2</sub> observation comparisons. CS and KM provided ATom and NOAA aircraft CO<sub>2</sub> observations and contributed interpretation of aircraft CO<sub>2</sub> observation comparisons. We furthermore acknowledge funding from the EU for the ERC project "ASICA" (grant number 649087) to Wouter Peters (Groningen University) and EU and NERC (UK) funding to Emanuel Gloor (University of Leeds), which contributed to the INPE Amazon greenhouse sampling program. All authors contributed to the writing, and have reviewed and approved the paper.

## **10** Competing interest

The authors declare that they have no conflict of interest.

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- 623 Appendix
- 624 As shown in Kalnay (2003):
- $RMSE^2 = R_{aircraft} + HP^aH^T$ (A.1)
- where  $R_{aircraft}$  is the aircraft observation error variance, and  $P^a$  is the posterior flux error
- 627 covariance. The H is linearized observation operator, which transfers posterior flux errors to
- 628 aircraft observation space, and  $H^T$  is its adjoint. In the Monte Carlo method, the postieror flux
- 629 error covariance  $P^a$  is approximated by:
- 630  $P^a = \frac{1}{nens} X^a X^{aT}$  (A.2)
- where  $X^a$  is the ensemble perturbations written as:
- 632  $X^a = x^a \bar{x}^a$  (A.3)
- where  $x^a$  is the ensemble posterior fluxes from Monte Carlo, and  $\bar{x}^a$  is the mean.
- 634 Therefore,  $HP^aH^T$  can be written as:
- 635  $HP^aH^T = \frac{1}{nens}[h(x^a) h(\bar{x}^a)][h(x^a) h(\bar{x}^a)]^T$  (A.4)
- The right hand side is the same as the definiation of  $RMSE_{MC}$  in the main text.
- 637 Therefore, when the posterior flux uncertainty estimated by Monte Carlo method represents the
- actual uncertainty in posterior fluxes, equation (A.1) can be written as:
- 639  $RMSE^2 = R_{aircraft} + RMSE_{MC}^2$  (A.5).
- 640 It is the same as equation (3) in the main text.





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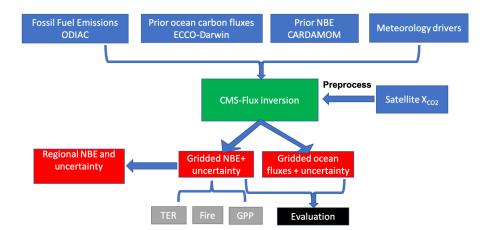


Figure: 1 Data flow diagram with the main processing steps to generate regional net biosphere change (NBE). TER: total ecosystem respiration; GPP: gross primary production. The green box is the inversion system. The blue boxes are the inputs for the inversion system. The red boxes are the data outputs from the system. The black box is the evaluation step, and the grey boxes are the future additions to the product.



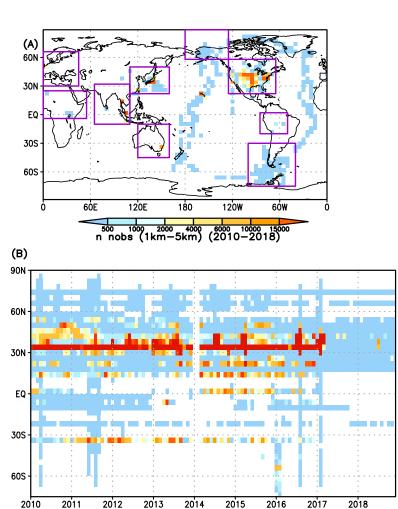


Figure: 2 The spatial and temporal distributions of aircraft observations used in evaluation of posterior NBE. (A) The total number of aircraft observations between 1–5 km between 2010–2018 at each  $4^{\circ}$  x  $5^{\circ}$ grid point. The rectangle boxes show the range of the nine sub regions. (B) The total number of monthly aircraft observations at each longitude as a function of time.

n nobs (1km-5km) (monthly)

1000 1200 1600 2000 2400 2800

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989 990

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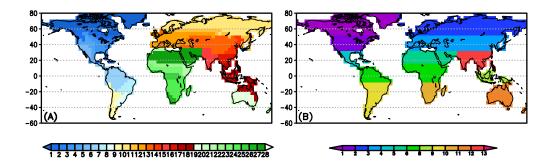


Figure: 3 Two types of regional masks used in calculating regional fluxes. The mask in (A) is based on a combination of condensed seven MODIS IGBP plant functional types, TRANCOM-3 regions (Gurney et al., 2004), and continents. The mask in (B) is based on latitude and continents.



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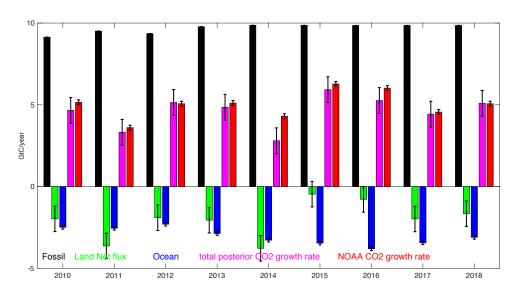


Figure: 4 Global flux estimation and uncertainties from 2010 –2018 (black: fossil fuel; green: posterior land fluxes; blue: ocean fluxes; magenta: estimated CO<sub>2</sub> growth rate; red: NOAA CO<sub>2</sub> growth rate).



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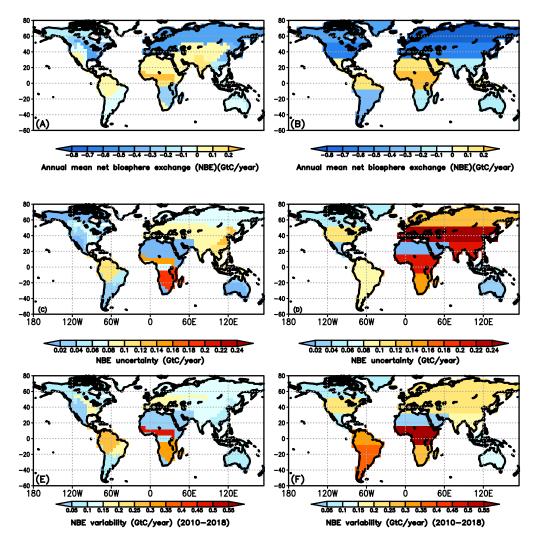


Figure: 5 Mean annual regional NBE (A and B), uncertainty (C and D), and variability between 2010–2018 (E and F) with two types of regional masks.



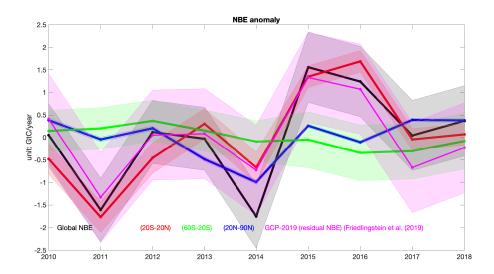


Figure: 6 The NBE interannual variability over the globe (black), the tropics (20°S–20°N), SH mid-latitudes (60°S–20°S), and NH mid-latitudes (20°N–9°0N). For reference, the residual net land carbon sink from GCP (Friedlingstein et al., 2019) and its uncertainty is also shown (magenta).



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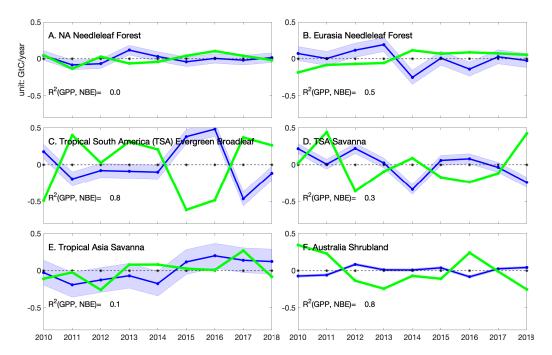


Figure: 7 The NBE interannual variability over six selected regions. Blue: annual NBE anomaly and its uncertainties. Green: annual GPP anomaly based on FLUXSAT.



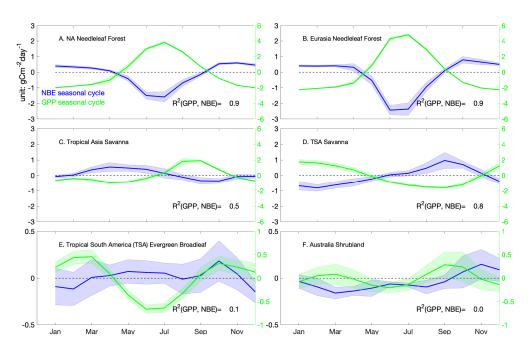
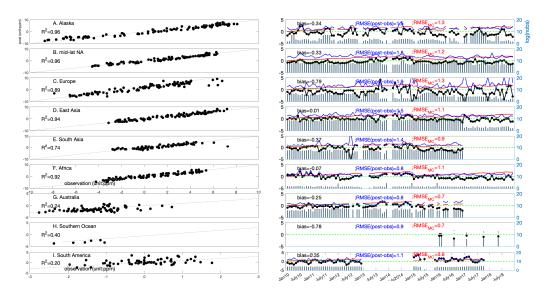


Figure: 8 Blue: climatological NBE seasonality over six selected regions shown in Figure 3A; blue shaded: NBE monthly uncertainty and variability (1-sigma) over nine years. Green and shaded: monthly mean GPP and its variability (1-sigma) over nine years. The names of each region are shown on individual subplots.





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Figure: 9 Comparison between posterior  $CO_2$  mole fraction and aircraft observations. Left panel: detrended posterior  $CO_2$  (y-axis) vs. detrended aircraft  $CO_2$  (x-axis) over nine regions. The dashed line is 1:1 line; right panel: black: the differences between posterior  $CO_2$  and aircraft  $CO_2$  as a function of time; blue: RMSE (unit: ppm); red: RMSE<sub>MC</sub>. The blue bar shows the number of aircraft observations (log scale) as a function of month.



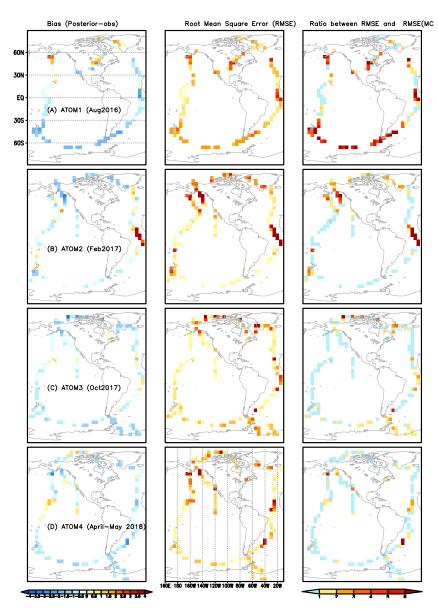


Figure: 10 Left column: the mean differences between posterior  $CO_2$  and aircraft observations from ATOM 1–4 aircraft campaigns between 1–5 km (A–D). Middle column: the Root Mean Square Errors (RMSE) between aircraft observations and posterior  $CO_2$  between 1–5 km. The color bar is the same as the left column. Right column: the ratio between RMSE and RMES $_{MC}$  based on ensemble  $CO_2$  from the Monte Carlo uncertainty estimation method.



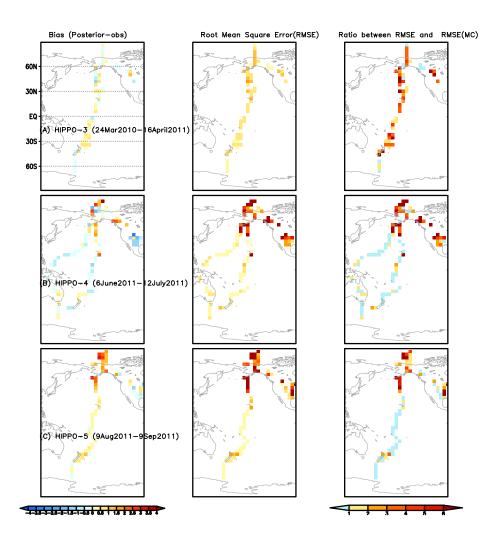


Figure: 11 Left column: the mean differences between posterior  $CO_2$  and aircraft observations from HIPPO 3-5 aircraft campaigns between 1–5 km (A–C) (unit: ppm). (unit: ppm). The time frame of each campaign is in the figure. Middle column: the Root Mean Square Errors (RMSE) between aircraft observations and posterior  $CO_2$  between 1–5 km (unit: ppm). The color bar is the same as the left column. Right column: the ratio between RMSE and RMSE<sub>MC</sub> based on ensemble  $CO_2$  from the Monte Carlo method.





## Table: 1 Configurations of the CMS-Flux atmospheric inversion system

	Model setup	Configuration	Reference
Inversion general	Spatial scale	Global	
setup	Spatial resolution Time resolution	4° latitude x 5° longitude monthly	
	Minimizer of cost function	L-BFGS	Byrd et al., 1994; Zhu et al., 1997
	Control vector	Monthly net terrestrial biosphere fluxes and ocean fluxes	
Transport model	Model name	GEOS-Chem and its adjoint	Suntharalingam et al., 2004
			Nassar et al., 2010 Henze et al., 2007
	Meteorological forcing	GEOS-5 (2010–2014) and GEOS-FP (2015–2019)	Rienecker et al., 2008

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## Table: 2 Description of the prior fluxes and assumed uncertainties in the inversion system

Prior fluxes	Terrestrial	Ocean fluxes	Fossil fuel emissions
	biosphere fluxes		
Model name	CARDAMOM-v1	ECCO-Darwin	ODIAC 2018
<b>Spatial resolution</b>	4° x 5°	0.5°	1° x 1°
Frequency	3-hourly	3-hourly	hourly
Uncertainty	Estimated from	100% same as Liu et al.	No uncertainty
·	CARDAMOM	(2017)	•
References	Bloom et al., 2006;	Brix et al, 2015; Carroll et al.,	Oda et al., 2016; 2018
	2020	2020	

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Table: 3 Description of observation and evaluation dataset. Data sources are listed in Table 7.

	Dataset name and version	References
Satellite X <sub>CO2</sub>	ACOS-GOSAT v7.3	O'Dell et al., (2012)
	OCO-2 v9	O'Dell et al., (2018)
Aircraft CO <sub>2</sub> observations	ObsPack OCO-2 MIP	CarbonTracker team (2019)
	HIPPO 3-5	Wofsy et al. (2011)
	ATOM 1-4	Wofsy et al.(2018)
	INPE	Gatti et al., (2014)
	ORCAS	Stephens et al., 2017
GPP	FLUXSAT-GPP	Joiner et al., (2018)





Table: 4 Latitude and longitude ranges for seven sub regions.

Region	Alaska	Mid-lat NA	Europe	East Asia	South Asia
Longitude	180°W–125° W	125°W–65°W	5°W–45°E	110°E–160°E	65°E–110°E
range					
Latitude	58°N–89°N	22°N-58°N	30°N-66°N	22°N-50°N	10°S-32°N
range					
Region	Africa	South	Australia	Southern	
_		America		Ocean	
Longitude	5°W-55°E	95°W-50°W	120°E–160°E	110°W–40°E	
range					
Latitude	2°N-18°N	20°S–2°N	45°S–10°S	80°S-30°S	
range					

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## **Table: 5 List of the data products.**

Product	Spatial resolution	Temporal resolution when applicable	Data format	Sample data description in the text
Total fossil fuel, ocean, and land fluxes	Global	Annual	csv	Figure 4 (section 4.1)
Climatology mean NBE, variability, and uncertainties	PFT and continents based 28 regions	N/A	CSV	Figure 5 (section 4.2)
	Geographic-based 13 regions		CSV	
Hemispheric NBE and uncertainties	NH (20°N-90°N), tropics (20°S- 20°N), and SH (60°S-20°S)	Annual	csv	Figure 6 (section 4.3)
NBE variability and uncertainties	PFT and continents based 28 regions	Annual	CSV	Figure 7 (section 4.3)
	Geographic -based 13 regions		CSV	
NBE seasonality and its uncertainties	PFT and continents based 28 regions	Monthly csv		Figure 8 (section 4.4)
	Geographic -based 13 regions		CSV	
Monthly NBE and uncertainties	PFT and continents based 28 regions	Monthly	CSV	N/A
	Geographic -based 13 regions		CSV	
Gridded NBE and uncertainties	4° (latitude) x 5° (longitude)	Monthly	NetCDF	N/A
Region masks	PFT and continents based 28 regions	N/A	csv	Figure 3 (section 2.4)
	Geographic -based 13 regions		csv	, 
Fluxes at a few selected flux tower sites	_	Monthly	csv	N/A





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Table: 6 The nine-year mean regional annual fluxes, uncertainties, and variability. Regions are based on the mask shown in Figure 5A (Figure 5.csv). Unit: GtC/year

are based on the mask shown in Figure 3A			
Region name (Figure4.csv)	Mean NBE	Uncertainty	Variability
NA shrubland	-0.14	0.02	0.05
NA needleleaf forest	-0.22	0.04	0.06
NA deciduous forest	-0.2	0.04	0.07
NA crop natural vegetation	-0.41	0.06	0.18
NA grassland	-0.04	0.03	0.03
NA savannah	0.03	0.02	0.03
Tropical South America (SA) evergreen broadleaf	0.04	0.1	0.28
SA savannah	-0.09	0.06	0.18
SA cropland	-0.07	0.03	0.07
SA shrubland	-0.03	0.02	0.08
Eurasia shrubland savanna	-0.44	0.07	0.14
Eurasia needleleaf forest	-0.41	0.07	0.12
Europe cropland	-0.46	0.09	0.16
Eurasia grassland	0.02	0.08	0.13
Asia cropland	-0.37	0.13	0.08
India	0.14	0.09	0.14
Tropical Asia savanna	-0.12	0.11	0.08
Tropical Asia evergreen broadleaf	-0.09	0.09	0.12
Australia (Aus) savannah grassland	-0.11	0.02	0.09
Aus shrubland	-0.07	0.01	0.05
Aus cropland	-0.01	0.01	0.03
African (Afr) northern shrubland	0.04	0.02	0.03
Afr grassland	0.03	0.01	0.01
Afr northern savanna	0.54	0.15	0.49
Afr southern savanna	-0.27	0.18	0.33
Afr evergreen broadleaf	0.1	0.07	0.09
Afr southern shrubland	0.01	0.01	0.01
Afr desert	0.06	0.01	0.04

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## 1095 Table: 7 Lists of data sources used in producing and evaluating posterior NBE product.

Data name	Data Source	
ECCO-Darwin	https://data.nas.nasa.gov/ecco	
ocean fluxes		
CARDAMOM	https://doi.org/10.25966/4v02-c391	
NBE and uncertainties		
ODIAC	http://db.cger.nies.go.jp/dataset/ODIAC/DL odiac2019.html	
GOSAT b7.3	https://oco2.gesdisc.eosdis.nasa.gov/data/GOSAT_TANSO_Level2/	
	ACOS_L2S.7.3/	
OCO-2 b9	https://disc.gsfc.nasa.gov/datasets?page=1&keywords=OCO-2	
ObsPack	https://www.esrl.noaa.gov/gmd/ccgg/obspack/data.php	
ATom 1-4	https://daac.ornl.gov/ATOM/guides/ATom merge.html	
HIPPO 3-5	https://www.eol.ucar.edu/field_projects/hippo	
INPE	https://www.esrl.noaa.gov/gmd/ccgg/obspack/data.php?id=obspack_	
	co2 1 INPE RESTRICTED v2.0 2018-11-13	
	and	
FLUXSAT-GPP	https://gs614-avdc1-pz.gsfc.nasa.gov/pub/tmp/FluxSat_GPP/	
Posterior NBE	https://doi.org/10.25966/4v02-c391	

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