1 Terrestrial ecosystem carbon flux estimated using GOSAT and OCO-2 XCO₂ re-

2 trievals

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Abstract

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In this study, both the Greenhouse Gases Observing Satellite (GOSAT) and the Orbiting Carbon Observatory 2 (OCO-2) XCO₂ retrievals produced by NASA Atmospheric CO₂ Observations from Space (ACOS) project (Version b7.3), are assimilated within the GEOS-Chem 4D-Var assimilation framework to constrain the terrestrial ecosystem carbon flux during Oct 1, 2014 to Dec 31, 2015. One inversion for the comparison, using in situ CO₂ observations, and another inversion as a benchmark for the simulated atmospheric CO₂ distributions of the real inversions, using global atmospheric CO₂ trend and referred as poor-man inversion, are also conducted. The estimated global and regional carbon fluxes for 2015 are shown and discussed. CO2 observations from surface flask sites and XCO₂ retrievals from TCCON sites are used to evaluate the simulated concentrations with the posterior carbon fluxes. Globally, the terrestrial ecosystem carbon sink (excluding biomass burning emissions) estimated from GOSAT data is stronger than that inferred from OCO-2 data, weaker than the in situ inversion, and matches the poor-man inversion to be the best. Regionally, in most regions, the land sinks inferred from GOSAT data are also stronger than those from OCO-2 data, and in North America, Asia, Europe, the carbon sinks inferred from GOSAT inversion are comparable to those from in situ inversion. For the latitudinal distribution of land sinks, the satellites-based inversions suggest a smaller boreal and tropical sink, but larger temperate sinks in both Northern and

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Southern Hemispheres than the in situ inversion. However, OCO-2 and GOSAT generally do not agree on which continent contains the smaller or larger sinks. Evaluations using flask and TCCON observations and the comparisons with in situ and poor-man inversions suggest that only GOSAT and the in situ inversions perform better than a poor-man's solution. GOSAT data can effectively improve the carbon flux estimates in Northern Hemisphere, while OCO-2 data, with the specific version used in this study, shows only slight improvement. The differences of inferred land fluxes between GOSAT and OCO-2 inversions in different regions are mainly related to the spatial coverage, the data amount, and the biases of these two satellites XCO₂ retrievals.

Keywords: Terrestrial ecosystem carbon flux, inversion, GOSAT, OCO-2, GEOS-Chem

1. Introduction

Atmospheric inverse modeling is an effective method for quantifying surface carbon fluxes at global and regional scales using the gradient of CO₂ measurements. Inversion studies based on in situ CO₂ observations agree well on global carbon budget estimates but differ greatly on regional carbon flux estimates and the partitioning of land and ocean fluxes as well, mainly due to the sparseness of observations in tropics, southern hemisphere oceans and the majority of continental interiors such as those in South America, Africa, and Boreal Asia (Peylin el al., 2013). Satellite observations offer an attractive means to constrain atmospheric inversions with their extensive spatial coverage over remote regions. Studies have shown that, theoretically, satellite observations, though with lower precision than in situ measurements, can improve the carbon flux estimates (Rayner and O Brien, 2001; Pak and Prather, 2001; Houweling et al., 2004; Baker et al., 2006; Chevallier et al., 2007; Miller et al., 2007; Kadygrov et al., 2009; Hungershoefer et al., 2010).

Satellite sensors designed specifically to retrieve atmospheric CO₂ concentrations, have been in operation in recent years. The Greenhouse Gases Observing Satellite (GOSAT) (Kuze et al., 2009), being the first satellite mission dedicated to observing CO₂ from space, was launched in 2009. The

National Aeronautics and Space Administration (NASA) launched the Orbiting Carbon Observa-52 tory 2 (OCO-2) satellite in 2014 (Crisp et al., 2017; Eldering et al., 2017). China's first CO₂ moni-53 toring satellite (TanSat) was launched in 2016 (Wang et al., 2017; Yang et al., 2017). These satel-54 lites measure near-infrared sunlight reflected from the surface in CO₂ spectral bands and the O₂ A-55 band to retrieve column-averaged dry-air mole fractions of CO₂ (XCO₂), aiming to improving the 56 estimation of spatial and temporal distributions of carbon sinks and sources. A number of inversions 57 have utilized GOSAT XCO2 retrievals to infer surface carbon fluxes (Basu et al., 2013; Maksyutov 58 et al., 2013; Saeki et al., 2013; Chevallier et al., 2014; Deng et al., 2014; Houweling et al., 2015; 59 Deng et al, 2016). Although large uncertainty reductions were achieved for regions which are un-60 61 der-sampled by in situ observations, these studies didn't give robust regional carbon flux estimates. 62 There are large spreads in regional flux estimates in some regions among these inversions. Furthermore, regional flux distributions inferred from GOSAT XCO2 data are significantly different from 63 those inferred from in situ observations. For instance, several studies using GOSAT retrievals re-64 ported a larger than expected carbon sink in Europe (Basu et al., 2013; Chevallier et al., 2014; Deng 65 et al., 2014; Houweling et al., 2015). The validity of this large Europe carbon sink derived from 66 GOSAT retrievals is in intense debate and efforts to improve the accuracy of Europe carbon sink 67 estimate are still ongoing (Reuter et al., 2014; Feng et al., 2016; Reuter et al., 2017). 68 69 Compared with GOSAT, OCO-2 has a higher sensitivity to column CO₂, much finer footprints 70 and more extended spatial coverage, and thus has the potential to better constrain the surface carbon fluxes (Eldering et al., 2017). Studies have used OCO-2 XCO₂ data to estimate carbon flux anoma-71 lies during recent El Nino events (Chatterjee et al., 2017; Patra et al., 2017; Heymann et al., 2017; 72 73 Liu et al., 2017). Nassar et al. (2017) applied OCO-2 XCO₂ data to infer emissions from large power plants. Miller et al. (2018) evaluated the potential of OCO-2 XCO₂ data in constraining re-74 gional biospheric CO₂ fluxes and found that in the current state of development, OCO-2 observa-75 tions can only provide a reliable constraint on CO₂ budget at continental and hemispheric scales. At 76

present, it is still not clear whether with the improved monitoring capabilities and better spatial coverage, current OCO-2 observations have a greater potential than GOSAT observations for estimating CO₂ flux at regional or finer scale, since the biases also affect the usefulness of satellite retrievals greatly. It is therefore important to investigate how current OCO-2 XCO₂ data differ from GO-SAT XCO₂ data in constraining carbon budget.

In this study, we evaluate the performance of GOSAT and OCO-2 XCO₂ data in constraining terrestrial ecosystem carbon flux. GOSAT and OCO-2 XCO₂ retrievals produced by the NASA Atmospheric CO₂ Observations from Space (ACOS) team are applied to infer monthly terrestrial ecosystem carbon sinks and sources from Oct, 2014 through December, 2015, using a 4D-Var scheme based on the GEOS-Chem Adjoint model (Henze et al., 2007). For comparisons, one inversion based on in situ measurements is conducted, and another simple one, which uses the global CO₂ trend as a benchmark for the simulated atmospheric CO₂ distributions of the real inversion, is also implemented. For simplicity, four inversions are referred as OCO-2 inversion, GOSAT inversion, in situ inversion and poor-man inversion, respectively. Inversion results are evaluated against surface flask CO₂ observations and Total Carbon Column Observing Network (TCCON) XCO₂ retrievals. This paper is organized as follows. Section 2 briefly introduces GOSAT and OCO-2 XCO₂ retrievals, surface observations and the inversion methodology. Inversion settings are described in Section 3. Results and discussions are presented in Section 4, and Conclusions are given in Section 5.

2. Data and Method

2.1 GOSAT and OCO-2 XCO2 retrievals

Developed jointly by the National Institute for Environmental Studies (NIES), the Japanese Space Agency (JAXA) and the Ministry of the Environment (MOE) of Japan, GOSAT was designed to retrieve total column abundances of CO₂ and CH₄. The satellite flies at a 666 km altitude in a sun-synchronous orbit with 98° inclination that crosses the equator at 12:49 local time. It covers the whole globe in three days and has a footprint of 10.5 km² at nadir. OCO-2 is NASA's first

mission dedicated to retrieving atmospheric CO_2 concentration. It flies at 705 km altitude in a sunsynchronous orbit with an overpass time at approximately 13:30 local time and a repeat cycle of 16 days. Its grating spectrometer measures reflected sunlight in three near-infrared regions (0.765, 1.61 and 2.06 μ m) to retrieve XCO_2 . OCO-2 has a footprint of 1.29×2.25 km² at nadir and acquires eight cross-track footprints creating a swath width of 10.3 km.

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Both GOSAT and OCO-2 XCO₂ products were created using the same retrieval algorithm, which is based on a Bayesian optimal estimation approach (Rogers et al., 2000; O Dell et al., 2011). The GOSAT and OCO-2 XCO₂ data used in this study are Version 7.3 Level 2 Lite products at the pixel level. The XCO₂ data from lite products are bias-corrected (Wunch et al., 2011). Before being used in our inversion system, the data are processed in three steps. First, the retrievals for the glint soundings over oceans have relatively larger uncertainty, thus the data over oceans are not used in our inversions (Wunch et al., 2017). Second, in order to achieve the most extensive spatial coverage with the assurance of using best quality data available, the XCO₂ data are filtered with two parameters, namely warn levels and xco2 quality flag, which are provided along with the XCO₂ data. All data with xco2 quality flag not equaling 0 are removed, the rest are divided into three groups according the value of warn_levels, namely group 1, group 2 and group 3. In group 1, the warn_levels are less than 8, in group 2, the warn_levels are greater than 9 and less than 12, and in group 3, those are greater than 13. Group 1 has the best data quality, followed by group 2, and group 3 is the worst. Third, the pixel data are averaged within the grid cell of 2°×2.5°, which is the resolution of the global atmospheric transport model used in this study. In each grid of $2^{\circ} \times 2.5^{\circ}$, only the groups of best data quality are selected and then averaged. The other variables like column averaging kernel, retrieval error and so on which are provided along with the XCO₂ product are also dealt with the same method. Figures 1a and 1b show the coverages and data amount of GOSAT and OCO-2 XCO₂ data during the study period after processing. The filtered GOSAT and OCO-2 retrievals are not evenly distributed spatially. Due to the cloud contamination, there are few retrievals in a large

portion of tropical land. In northern high latitude area, especially in boreal regions, due to the low soar zenith angle, available satellite retrievals are very sparse.

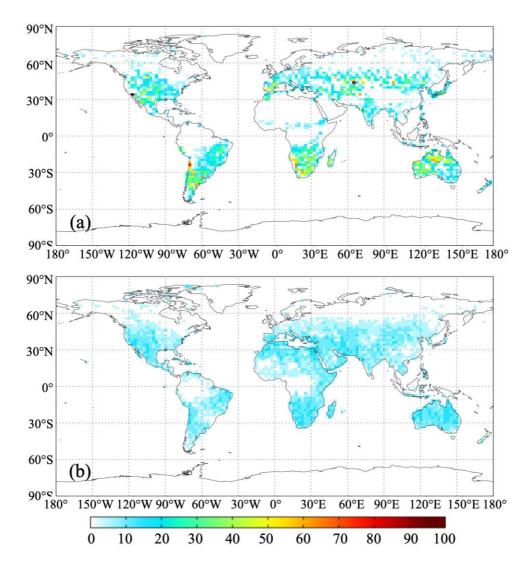


Figure 1. Data amount of each grid cell (2°×2.5°) of ACOS XCO₂ used in this study (a, GOSAT; b, OCO-2)

2.2 Surface observations and TCCON XCO2 retrievals

Surface CO₂ observations are from the obspack_co2_1_CARBONTRACKER_CT2016_2017-02-06 product (ObsPackCT2016) (CarbonTracker Team, 2017), which was the observation data used in CarbonTracker 2016 (Peters et al., 2007, with updates documented at http://carbontracker.noaa.gov). It is a subset of the Observation Package (ObsPack) Data Product (ObsPack, 2016), and contains a collection of discrete and quasi-continuous measurements at surface, tower

and ship sites contributed by national and universities laboratories around the world. In this study, in situ measurements from 78 sites provided by this product are used for inversion. Among these 78 sites, there are 56 flask sites, of which 52 sites are selected to evaluate the posterior CO₂ concentrations (selection criteria given in Section 4.1.1).

TCCON is a network of ground-based Fourier Transform Spectrometers that measure direct near-infrared solar absorption spectra. Column-averaged abundances of atmospheric constituents including CO₂, CH₄, N₂O, HF, CO, H₂O, and HDO are retrieved through these spectra. We use XCO₂ retrievals from 13 stations from TCCON GGG2014 dataset (Blumenstock et al., 2017; Deutscher et al., 2017; Griffith et al., 2017a, b; Kivi et al., 2017; Morino et al., 2017; Notholt et al., 2017a, b; Sherlock et al., 2017; Sussmann and Rettinger, 2017; Warneke et al., 2017; Wennberg et al., 2017a, b). The names of the 13 stations are Bialystok (Bial), Bremen (Brem), Orleans (Orle), Garmisch (Garm), Darwin (Darw), Izana (Izan), Ny Alesund (Ny_A), Lamont (Lamo), Lauder (Laud), Park Falls (Park), Sodankyla (Soda), Tsukuba (Tsuk), and Wollongong (Woll). The locations of in situ sites and 13 TCCON stations are shown in Figure 2.

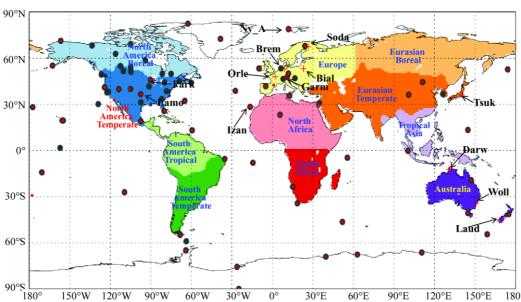


Figure 2. Distributions of the observation sites used in this study. Gray solid circles are surface sites used in the in situ inversion, red points and red cross marks are surface flask and TCCON sites used for evaluations, respectively, the shaded area shows the 11 TRANSCOM regions

2.3 GEOS-Chem 4DVAR assimilation framework

2.3.1 GEOS-Chem model

GEOS-Chem model (http://geos-chem.org) is a global three-dimensional chemistry transport model (CTM), which is driven by assimilated meteorological data from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office (GMAO) (Rienecker et al., 2008). The original CO₂ simulation in the GEOS-Chem model was developed by Suntharalingam et al. (2004) and accounts for CO₂ fluxes from fossil fuel combustion and cement production, biomass burning, terrestrial ecosystem exchange, ocean exchange and biofuel burning. Nassar et al. (2010) updated the CO₂ simulation with improved inventories. In addition to the inventories in earlier version, the new CO₂ fluxes includes CO₂ emissions from international shipping, aviation (3D) and the chemical production of CO₂ from CO oxidation throughout the troposphere. In most other models, the oxidation of CO was treated as direct surface CO₂ emissions. The details of the CO₂ simulation and the CO₂ sinks/sources inventories could be found in Nassar et al. (2010). The version of GEOS-Chem model used in this study is v8-02-01.

2.3.2 GEOS-Chem adjoint model

An adjoint model is used to calculate the gradient of a response function of one model scalar (or cost function) with respect to a set of model parameters. The adjoint of the GEOS-Chem model was first developed for inverse modeling of aerosol (or their precursors) and gas emissions (Henze et al., 2007). It has been implemented to constrain sources of species such as CO, CH₄, and O₃ with satellite observations (Kopacz et al., 2009, 2010; Jiang et al., 2011; Wecht et al., 2012; Parrington et al., 2012). Several studies have successfully used this adjoint model to constraint carbon sources and sinks with surface flask measurements of CO₂ mixing ratio and space-based XCO₂ retrievals (Deng et al., 2014; Liu et al., 2014; Deng et al., 2016; Liu et al., 2017).

2.3.3 Inversion method

In the GEOS-Chem inverse modeling framework, the 4D-Var data assimilation technique is

employed for combining observations and simulations to seek a best optimal estimation of the state of a system. The scaling factors are applied to the carbon flux components to be optimized monthly in each model grid point. This approach seeks the scaling factors of the carbon flux that minimize the cost function, J, given by:

$$J(c) = \frac{1}{2} \sum_{i=1}^{N} \left(XCO_{2,i}^{m} - XCO_{2,i}^{obs} \right) S_{obs,i}^{-1} \left(XCO_{2,i}^{m} - XCO_{2,i}^{obs} \right) + \left(\frac{1}{2} (c - c_a) S_c^{-1} (c - c_a) \right)$$
(1)

where N is total number of satellite XCO₂ observations; XCO₂^m and XCO₂^{obs} are modeled and observed total column averaged dry air mole faction of CO₂ respectively; c_a is the prior scaling factor of the carbon flux, which is typically set as unity; S_{obs} is the model-data mismatch error covariance matrix; S_c is the scaling factor error covariance matrix. The gradients of the cost function with respect to scaling factors calculated with the adjoint model are supplied to an optimization routine (the L-BFGS-B optimization routine; Byrd et al., 1995; Zhu et al., 1994), and the minimum of the cost function is sought iteratively.

For the modeled CO₂ column to be comparable with the satellite XCO₂ retrievals, the modeled CO₂ concentration profile should be first mapped into the satellite retrieval levels and then convoluted with retrieval averaging kernels. The modeled XCO₂ is computed by:

$$XCO_2^m = XCO_2^a + \sum_i h_i a_i (A(x) - y_{a,i})$$
 (2)

where j denotes retrieval level, x is the modeled CO₂ profile; A(x) is a mapping matrix; XCO₂^a is prior XCO₂, h_j is pressure weighting function, a_j is the satellite column averaging kernel and y_a is the prior CO₂ profile for retrieval. These last four quantities are provided from ACOS Version 7.3 Level 2 Lite products.

3. Inversion settings

In this study, the GEOS-Chem model was run in a horizontal resolution of 2°×2.5° for 47 verti-

cal layers. Three inversions, using GOSAT data, OCO-2 data, and in situ measurements, are conducted from Oct 1, 2014 to December 31, 2015, respectively. Poor-man inversion, based on global atmospheric CO₂ trend and using poor-man's method (Chevallier et al, 2009, 2010), is also conducted. The posterior dry air mole fraction of CO₂ on Oct 1, 2014 from CT2016 product is taken as the initial concentration. The first three months are taken as the spin-up period. The prior carbon fluxes used in this study include fossil fuel CO₂ emissions, biomass burning CO₂ emissions, terrestrial ecosystem carbon exchange and CO₂ flux exchange over the sea surface. Fossil fuel emissions are obtained from CT2016, which is an average of Carbon Dioxide Information Analysis Center (CDIAC) product (Andres et al., 2011) and Open-source Data Inventory of Anthropogenic CO₂ (ODIAC) emission product (Oda and Maksyutov, 2011). The biomass burning CO₂ emissions are also taken from CT2016, which are the average of the Global Fire Emissions Database version 4.1 (GFEDv4) (van der Werf et al., 2010; Giglio et al., 2013) and the Global Fire Emission Database from NASA Carbon Monitoring System (GFED_CMS). The 3-hourly terrestrial ecosystem carbon exchanges are from the Carnegie-Ames-Stanford Approach (CASA) model GFED4.1 simulation (Potter el al., 1993; van der Werf et al., 2010). CO₂ exchanges over the ocean surface are from the posterior air-sea CO₂ flux of CT2016. It is noted that the fossil fuel emissions and the biomass burning emissions in our inversions are kept intact. Both terrestrial ecosystem CO₂ exchanges and ocean flux are optimized in our inversions.

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An efficient computational procedure for constructing non-diagonal scaling factor error covariance matrix which accounts for the spatial correlation of errors is implemented (Single et al., 2011). The construction is based on the assumption of exponential decay of error correlations. Other than forming covariance matrix explicitly, multiple-dimensional correlations are represented by tensor products of one-dimensional correlation matrices along longitude and latitudinal directions. For the two inversions, the scale lengths assigned along longitudinal and latitudinal directions are 500 km

and 400 km for terrestrial ecosystem exchange and 1000 km and 800 km for ocean exchange, respectively. No correlations between different types of fluxes are assumed. The temporal correlations are also neglected. Global annual uncertainty of 100% and 40% are assigned for terrestrial ecosystem and ocean CO₂ exchanges, respectively (Deng and Chen, 2011). Accordingly, the uncertainty of scaling factor for the prior land and ocean fluxes in each month at the grid cell level are assigned to 3 and 5, respectively.

3.1 Inversions using satellite XCO₂ retrievals

The observation error covariance matrix is constructed using the retrieval errors, which are provided along with the ACOS XCO₂ data. Observation errors are assumed to be uncorrelated at model grid level. To account for the correlated observation errors, as shown in section 2.1, the pixel level retrieval errors are filtered and averaged to the model grid level, and then inflated by a factor of 1.9 to ensure the chi-square testing of χ^2 value to be close to 1 (Tarantola, 2004; Chevallier et al., 2007).

3.2 Inversion using in situ measurements

As described in section 2.2, surface CO₂ observations from 78 sites including flask samples and by quasi-continuous analyzer are adopted in this inversion. These data are selected from data collection of the ObsPackCT2016. The observation uncertainties of the 78 sites are also obtained from this product, which account for both the measurement and representative errors (Peters et al., 2007, with updates documented at http://carbontracker.noaa.gov). An examination for the differences between observations and forward model simulation was conducted (data not shown), and the results shows that observation uncertainties from CT2016 represents well with the model-data mismatch errors of GEOS-Chem model. In addition, we neglect correlations between observations and assume a diagonal observation error covariance matrix.

3.3 Poor-man inversion

A baseline inversion, which was introduced by Chevallier et al. (2009, 2010) as a poor-man's

Usually, the posteriori fluxes are evaluated by the improvement on the simulated CO₂ mixing ratios.

Since the global CO₂ trend can be accurately estimated from marine sites, it is important to assess

method, is implemented to evaluate satellite retrievals and in situ measurements based inversions.

whether the inverted flux can capture more information than this trend. In this baseline inversion,

the ocean flux is kept identical to the prior ones. The poor-man's inverted land flux F_{pm} at location

(x, y) and at time t is defined as:

$$F_{pm}(x, y, t) = F_{prior}(x, y, t) + k \times \sigma(x, y, t)$$
(3)

259 where F_{prior} is the prior flux, σ is the uncertainty of the prior flux, k is a coefficient, it can be solved 260 directly from the formula (3) as

$$k = \left(\sum F_{pm}(x, y, t) - \sum F_{prior}(x, y, t)\right) / \sum \sigma(x, y, t)$$
(4)

where $\sum F_{pm}(x, y, t)$ equals the global total land flux, which can be calculated from the observed annual global CO₂ growth rate, global annual fossil fuel and biomass burning emissions, and ocean flux. In this study, the observed annual global CO₂ growth rate is from the Global Monitoring Division (GMD) of NOAA/Earth System Research Laboratory (ESRL) (Ed Dlugokencky and Pieter Tans, NOAA/ESRL, www.esrl.noaa.gov/gmd/ccgg/trends/). The annual global CO₂ growth rate is 2.96 ppm in 2015, which is converted to 6.28 PgC yr⁻¹ for the poor-man's global total by multiplying by a factor of 2.123 PgC ppm⁻¹.

4. Results and Discussions

4.1 Evaluation for the inversion results

4.1.1 Flask observations

As shown in section 2.2, Flask observations from 52 sites are used to evaluate the inversion results. Actually, there are much more flask observations in the dataset. When there are more than one flask dataset for one site, we give priority to that from NOAA/ESL or that with more consistent records. There are 56 sites with available flask observations for evaluation. In addition, during the

evaluations, we find that GEOS-Chem model is unable to capture the variations of CO₂ mixing ratios at HPB, HUN, SGP and TAP sites, where the standard deviations of the deviations between the observed and modeled mixing ratio are larger than 5 ppm. Therefore, we exclude these four sites and use the rest 52 flask sites (shown in Figure 2) to evaluate the posterior mixing ratios. The GEOS-Chem model is driven with the prior flux and the four posterior fluxes to obtain the prior and posterior CO₂ mixing ratios. The simulated CO₂ mixing ratios are sampled at each observation site and within half an hour of observation time.

Table 1 shows a summary of comparisons of the simulated CO₂ mixing ratios against the flask measurements. The mean difference between the prior CO₂ mixing ratio and the flask measurements is 0.93 ppm, with a standard deviation of 2.3 ppm. All four inversions show improvement in posterior concentrations with reductions of biases. Not surprisingly, in situ inversion, using surface observations which include all the flask measurements used for evaluation, shows the best improvement in posterior CO₂ mixing ratio with the largest reduction of bias and standard deviation. GOSAT inversion achieves almost the same reductions of standard deviation as in situ inversion. OCO-2 inversion gives larger bias and standard deviation than in situ and GOSAT inversions. Poor-man inversion effectively reduces the bias but with little improvement in the reduction of standard deviations.

Figure 3 shows the biases at each observation site in different latitudes. It could be found that the biases between the simulations and the observations in the northern hemisphere are significantly larger than those in southern hemisphere since the carbon flux distribution of the northern hemisphere is more complex than that of the southern hemisphere. When the prior flux is used, almost all sites in the northern hemisphere have significant positive deviations, with an average of 1.7 ppm, while in the southern hemisphere, the deviations are very small, with an average bias of only -0.08 ppm; when using the posteriori flux from OCO-2 inversion, the deviations in most northern hemisphere sites are slightly reduced, with an average deviation of 0.85 ppm, while in the southern hemisphere, at most sites, the biases increase by variable amounts, with a mean of -0.13 ppm; when using the posterior

flux from GOSAT inversion, the deviations are significantly reduced to 0.04 ppm in the northern hemisphere but further increased to -0.55 ppm in the southern hemisphere. In situ inversion shows similar improvement in Northern Hemisphere as GOSAT inversion does, but also with little improvement in Southern Hemisphere. Though poor-man inversion effectively reduces the global bias, it shows largest negative biases in Southern Hemisphere and moderate positive biases (close to OCO-2 inversions) in Northern Hemisphere, indicating that the improvements of poor-man inversion for posterior concentrations are very limited. These suggest that GOSAT and in situ inversions can effectively improve the carbon fluxes estimate in the northern hemisphere, but overestimate the land sinks in the southern hemisphere.

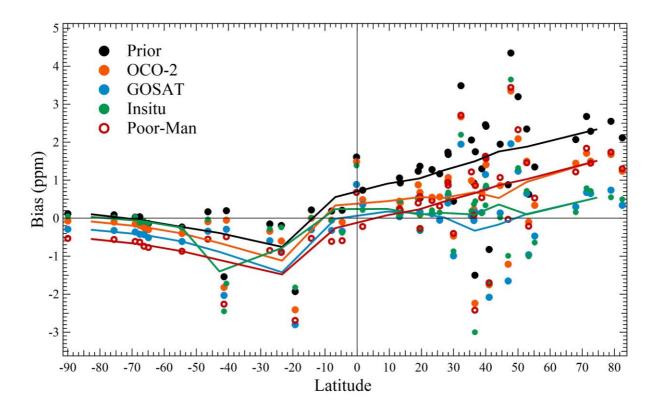


Figure 3. Biases of the simulated CO₂ mixing ratios against the flask measurements in different latitudes (positive/negative biases represent modeled concentration being greater/less than the observed, the different color lines are the smooth of the corresponding marks)

4.1.2 TCCON observations

We also use data from 13 TCCON sites (Figure 2) to evaluate our inversion results. The simu-

lated CO₂ concentrations at 47 vertical levels are mapped onto 71 TCCON levels. Following the approach of Wunch et al. (2011), using prior profiles and the averaging kernel from the TCCON dataset, we calculated the modeled XCO₂ values at 13 TCCON sites. It should be noted that the comparisons of posterior XCO₂ from GOSAT and OCO-2 inversions with TCCON data are not fully independent since the TCCON data were used in the bias-correction scheme of both GOSAT and OCO-2 products (Wunch et al., 2011). Table 1 also shows the comparison of modeled XCO₂ with TCCON observations. The mean difference between prior XCO₂ and TCCON retrievals is 1.16 ppm, with a standard deviation of 1.3 ppm. GOSAT inversion performs the best with the largest reductions of bias and standard deviation. Though OCO-2 inversion shows improvement in the reduction of standard deviation, it gives a relatively large bias for posterior XCO₂. In situ inversion has the same reduction of standard deviation as GOSAT inversion. Poor-man inversion reduces the bias to 0.49 ppm and gives slight improvement in reducing standard deviation of posterior XCO₂.

Figure 4 shows the bias at each TCCON site. Obviously, the biases at all TCCON sites are positive when using the prior fluxes, ranging between 0.3 and 2.6 ppm. The biases at the sites in the northern temperate and boreal areas are all above 1.5 ppm except for the Lamo site. GOSAT and in situ inversions significantly reduce the biases at most sites. However, in Northern Hemisphere, the biases at those sites remain relatively large. Since GOSAT and in situ inversions show evident improvement at flask sites in Northern Hemisphere, the remaining large biases at TCCON sites may be also related to the biases of TCCON retrievals (Wunch et al, 2010; Messerschmidt et al, 2011). OCO-2 and poor-man inversions show slight improvement in the reduction of biases at most sites and rather large biases still remain.

Overall, it also could be found from Table 1 that only in situ inversion beats the poor-man inversion on all 4 statistics, followed by GOSAT inversion, which beats the poor-man on 3 statistics, indicating that in situ measurements have the best performance among all inversions, and GOSAT retrieval have similar performance as in situ data.

Table 1. Statistics of the model-data mismatch errors at the 52 surface flask sites and the 13 TCCON sites (ppm)

	Flask		TCCON		
	Bias	Stdev	Bias	Stdev	
Prior	0.93	2.30	1.16	1.30	
OCO-2	0.33	2.15	0.80	1.08	
GOSAT	-0.19	2.05	0.22	1.04	
In situ	-0.03	2.04	0.38	1.04	
Poor-man	0.14	2.28	0.49	1.25	

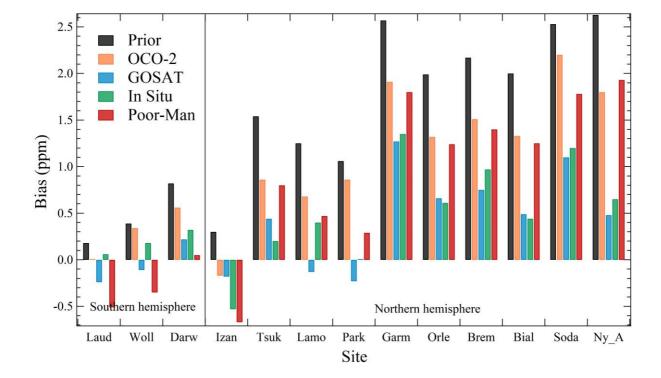


Figure 4. The biases between the modeled and observed XCO₂ at the 13 TCCON sites

4.2 Global carbon budget

Table 2 presents the global carbon budgets in 2015 from four inversions. The global land sinks inferred by GOSAT and OCO-2 XCO₂ retrievals are -3.48 and -2.94 PgC yr⁻¹, respectively, which

are both larger than the prior value, and lower than the estimate from the in situ inversion. The differences of ocean fluxes among a priori and two inversions are small since we don't assimilate XCO₂ data over ocean. The global net flux from the poor-man inversion is inferred from the global annual CO₂ growth rate, which represents relatively accurately the net carbon flux added into atmosphere. It could be found that the global net flux from GOSAT inversion is the closest to the poor-man inversion estimate, while that from OCO-2 inversion is higher and the in situ inversion estimate is lower than the poor-man estimate, indicating that GOSAT inversion has the best estimates for the land and ocean carbon uptakes, while those from in situ inversion are overestimated, and those from OCO-2 inversion might be underestimated.

Table 2. Global carbon budgets estimated by the OCO-2 and GOSAT inversions in this study as well as those from the prior fluxes, in situ and poor-man inversions (PgC yr⁻¹)

	Prior	OCO-2	GOSAT	In situ	Poor-man
Fossil fuel and industry	9.84	9.84	9.84	9.84	9.84
Biomass burning emissions	2.20	2.20	2.20	2.20	2.20
Land sink	-2.50	-2.94	-3.48	-3.63	-3.35
Ocean sink	-2.41	-2.44	-2.45	-2.41	-2.41
Global net flux	7.13	6.66	6.11	6.00	6.28

4.3 Regional carbon flux

Figure 5 shows the distributions of annual land and ocean carbon fluxes (excluding fossil fuel and biomass burning carbon emissions, same thereafter) of the prior and the estimates using GOSAT and OCO-2 data. It could be found that compared with the prior fluxes, the carbon sinks in Central America, south and northeast China, east and central Europe, south Russia and east Brazil are obviously increased in GOSAT inversion. Except for east Brazil, the land sinks in those areas in OCO-2 inversion are also increased, but much weaker than those in GOSAT inversion, and in east Brazil, it turns to a significant carbon source. In contrast, in east and central Canada, north Russia, north Europe, west Indo-China Peninsula, north Democratic Republic of the Congo and west Brazil, their

carbon sources are significantly increased in both GOSAT and OCO-2 inversions. In east and central Canada, north Europe and west Brazil, there are much stronger carbon sources in OCO-2 inversion.

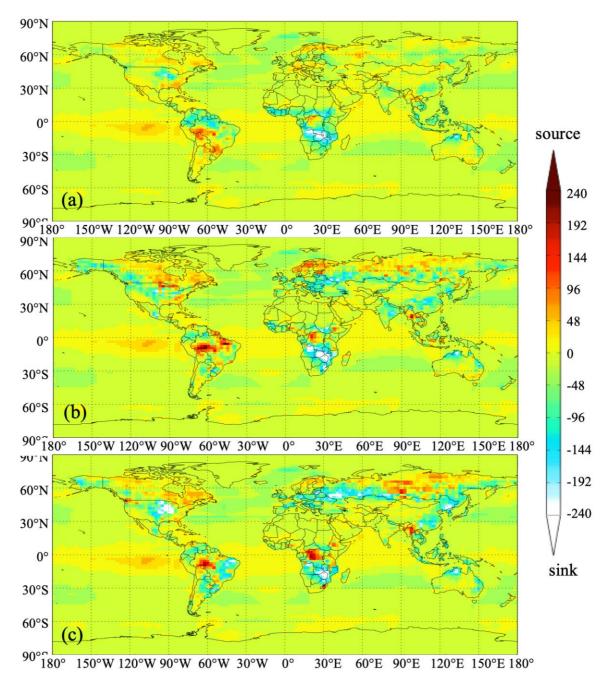


Figure 5. Distributions of annual land and ocean carbon fluxes a) prior flux and posterior fluxes based on (b) OCO-2 and (c) GOSAT data (gC m⁻²yr⁻¹)

To better investigate the differences between GOSAT and OCO-2 inversions as well as their differences with two other inversions, we aggregate the prior and inferred land fluxes into 11 TRANS-COM land regions (Gurney et al., 2002) as shown in Figure 2. Figure 6 shows aggregated annual land

surface fluxes from the prior and inversions for the 11 land regions. Clearly, in most regions, the land sinks inverted based on GOSAT data are stronger than those inferred from OCO-2 data, especially in the Temperate and Tropical Lands. For example, in South America Temperate, the estimated land sink based on GOSAT data is about 4 times as large as the OCO-2 inversions; in North America Temperate and Tropical Asia, the carbon sinks of GOSAT experiment is about twice that of the OCO-2 inversions; and in South America Tropical, the OCO-2 inversion result is a carbon source of 0.19 PgC yr⁻¹, while GOSAT inversion gives a weak sink of -0.05 Pg C yr⁻¹. The total sinks of the Temperate/Tropical Lands optimized using GOSAT and OCO-2 XCO₂ retrievals are -2.95/-0.36 and -2.59/-0.20 Pg C yr⁻¹, respectively (Table 3). In Northern Boreal Land, the total carbon sinks inverted with GOSAT and OCO-2 data are comparable. However, the two XCO₂ data have opposite performances in two northern boreal regions, namely in Eurasian Boreal, the inverted land sink with GOSAT is stronger than that with OCO-2; while in North America Boreal, it is the opposite.

For different continents (Table 3), in Asia and Australia, their carbon sinks inverted from GOSAT and OCO-2 data are comparable. In North America, South America and Europe, the land sinks in GOSAT inversion are much stronger than those in OCO-2 inversion. Especially in South America, the GOSAT inversion result is a strong carbon sink (-0.51 Pg C yr⁻¹), while in OCO-2 inversion, it is a weak carbon source (0.06 Pg C yr⁻¹). Conversely, in Africa, the land sink estimated with GOSAT data is much weaker than those from OCO-2 data, the former (-0.59 Pg C yr⁻¹) being only about the half of the latter (-1.13 Pg C yr⁻¹).

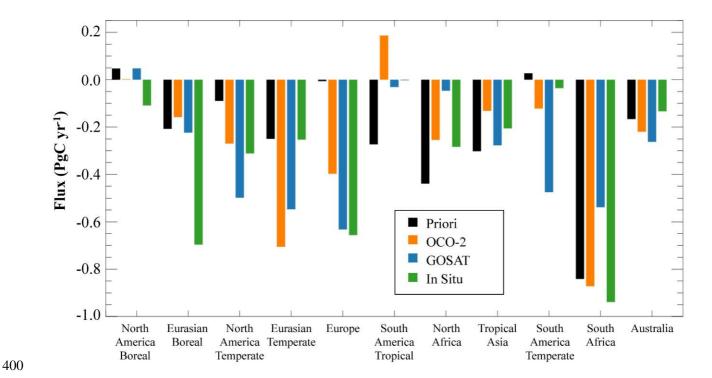


Figure 6. Aggregated annual land fluxes of the 11 TRANSCOM land regions

Table 3. The prior and posterior fluxes in six continents and boreal, temperate and tropical lands (PgC yr⁻¹)

Regions	Prior	OCO-2	GOSAT	In situ
North America	-0.04	-0.27	-0.45	-0.42
South America	-0.25	0.06	-0.51	-0.04
Europe	-0.01	-0.40	-0.63	-0.66
Asia	-0.76	-0.99	-1.05	-1.16
Africa	-1.28	-1.13	-0.58	-1.22
Australia	-0.17	-0.22	-0.26	-0.13
Northern Boreal Land	-0.16	-0.16	-0.18	-0.81
Northern Temperate Land	-0.35	-1.37	-1.68	-1.22
Tropical Land	-1.01	-0.20	-0.36	-0.49
Southern Temperate Land	-0.98	-1.21	-1.28	-1.11

Compared with the in situ inversion, in the boreal regions, the land sinks estimated from GOSAT and OCO-2 inversions are much weaker than those from in situ inversion, especially in the Eurasian Boreal, the land sink estimated by in situ inversion is more than two times larger than the estimates

of GOSAT and OCO-2 inversions. In the tropical land, the total land sinks inferred from both GOSAT and OCO-2 inversions are weaker than those from the in situ inversion, but in different regions, the situations are different. In the Temperate lands, except for Europe and south Africa, the land sinks from GOSAT and OCO-2 inversions are much stronger than those from the in situ inversion. For example, in South America Temperate, GOSAT inversion shows a strong carbon sink, while in situ inversion shows a weak source. For different continents, in North America, Asia, Europe, the carbon sinks inferred from GOSAT inversion are comparable to those from in situ inversion, while in South America and Africa, the carbon sinks inferred from OCO-2 inversion are much closer to the in situ inversion.

Compared with the prior fluxes, the inferred land fluxes in Northern Temperate regions have the largest changes, followed by those in Tropical regions and Southern Temperate lands, while in boreal regions, the changes are the smallest. As shown in Table 4, for different TRANSCOM regions and different XCO₂ used, the changes of carbon fluxes have large differences. Since the same setup used in these two inversions and the same algorithm adopted for retrieving XCO₂ from GOSAT and OCO-2 measurements, the different impacts of XCO₂ data on land sinks may be related to the spatial coverage and the amount of data in these two XCO₂ datasets. As shown in Figure 1, in different latitude zones, the spatial coverage and the data amount of GOSAT and OCO-2 have large differences. Statistics show that the amount of data is largest in northern temperate land, followed by southern temperate land and tropical land, and least in northern boreal regions, corresponding to the magnitude of changes of carbon fluxes in these zones. For one specific zone, the different impacts of these two XCO₂ datasets may be also related to their data amount. For example, in northern temperate land, GOSAT has more XCO₂ data than OCO-2. Accordingly, the change of carbon flux caused by GOSAT is larger than that caused by OCO-2. Conversely, in Tropical Land, OCO-2 has more data than GO-SAT, and as shown before it has more significant impact on the land sink. This relationship could also be found in each TRANSCOM region. Figure 5 gives a relationship between the XCO₂ data amount ratios of GOSAT to OCO-2 and the land sinks absolute change ratios caused by GOSAT to OCO-2 for 11 TRANSCOM land regions. Obviously, except for North and South Africa, there is a significant linear correlation (R=0.95) between these two ratios, suggesting that with more XCO₂ data, the more carbon flux relative to the prior flux is changed. In North Africa, we find that OCO-2 has better spatial coverage and more data than GOSAT, as shown in Figure 1. Although the differences mainly occur in the Sahara where the carbon flux is very weak, but near the equatorial region where the carbon flux is large, OCO-2 still has more data than GOSAT. In southern Africa, both XCO₂ have good spatial coverage, the amount of GOSAT data is about 1.5 times that of OCO-2, but the changes in the carbon flux caused by GOSAT is about 10 times that of OCO-2. The large ratio of carbon change is mainly due to the relatively small carbon change from OCO-2 inversion.

Table 4. Differences between the inferred and the prior carbon fluxes, the data amount of XCO₂ and the deviations between the modeled with prior flux and satellite retrieved XCO₂ in different regions

Region	Flux changed (Pg C yr ⁻¹)*		XCO ₂ data amount		Deviations (ppm)**	
	OCO-2	GOSAT	OCO-2	GOSAT	OCO-2	GOSAT
North America Boreal	-0.05	0	1143	639	0.6	1.41
North America Temperate	-0.18	-0.41	2390	3163	0.52	0.93
South America Tropical	0.46	0.24	800	421	-0.89	0.43
South America Temperate	-0.15	-0.5	1711	3500	0.02	0.54
North Africa	0.19	0.39	3208	674	0.12	-0.19
South Africa	-0.03	0.3	2057	3060	0.17	0.33
Eurasian Boreal	0.05	-0.02	1714	1339	0.47	1.5
Eurasian Temperate	-0.46	-0.3	5323	4782	0.46	0.82
Tropical Asia	0.17	0.03	726	550	-0.43	0.34
Australia	-0.05	-0.1	2011	3110	0.18	0.67
Europe	-0.39	-0.63	1604	2106	0.28	1.35
Global land	-0.44	-0.98	22687	23344	0.22	0.79
Northern Boreal Land	0.005	-0.02	2857	1978	0.52	1.47
Northern Temperate Land	-1.03	-1.33	9317	10051	0.45	0.96
Tropical Land	0.82	0.66	4734	1645	-0.08	0.13
Southern Temperate Land	-0.23	-0.3	5779	9670	0.11	0.6

^{*} Differences between posterior and prior flux

^{**} Deviations between the modeled XCO₂ with prior flux and satellite retrieved XCO₂

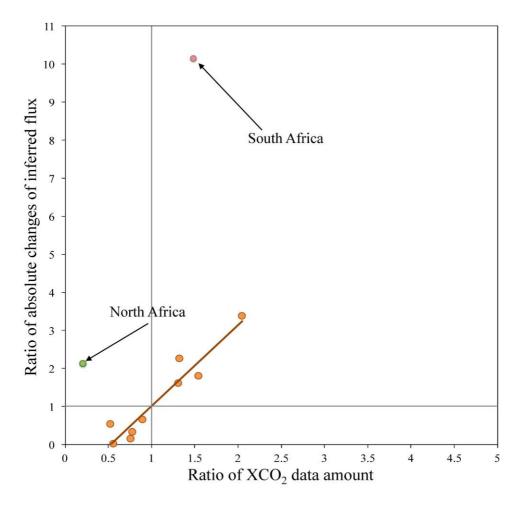


Figure 7. Scatter plot for the ratio of GOSAT to OCO-2 XCO₂ data amount versus the ratio of absolute changes of the land sinks caused by GOSAT to OCO-2 in the 11 TRANSCOM land regions

In addition to the data amount, the mismatches between the simulated CO₂ concentrations using prior fluxes and the satellite retrievals could be used to examine the performances of OCO-2 and GOSAT retrievals in different regions. Usually, a large model-data mismatch will impose strong constraint on the prior flux in inversions. Therefore, we compare the mismatches in OCO-2 and GOSAT inversions. The results are grouped global land and into the 11 TRANSCOM land regions, as shown in Table 4. The global land mean difference between modeled XCO₂ and the OCO-2 and GOSAT retrievals are 0.22 and 0.79 ppm, respectively, indicating that the GOSAT retrieval would have stronger constraint on the prior fluxes. In most TRANSCOM regions except North Africa, the mismatches in GOSAT inversion are positive and larger than those of OCO-2 inversion. In Tropic Asia and South America Tropic, the sizable negative mismatches in OCO-2 inversion could account

for a weak inverted carbon sink and an inverted carbon source in these two regions, while in North Africa, the negative mismatch in GOSAT inversion may explain why a rather weak sink is inverted for this region. The difference of mismatch between OCO-2 and GOSAT inversions exhibits rather large spread, ranging from 0.16 to 1.33 pm, indicating the biases of two satellite XCO₂ retrievals differ greatly.

Table 5. Statistics of the OCO-2 and GOSAT retrievals uncertainties against the TCCON retrievals

		OCO-2			GOSAT		
	Bias (ppm)	Stdev (ppm)	N. of Obs.	Bias (ppm)	Stdev (ppm)	N. of Obs.	
Bial	0.91	1.47	21	0.06	1.35	29	
Darw	0.75	0.85	43	-0.41	1.62	44	
Garm	-0.10	2.97	14	0.73	2.02	35	
Lamo	0.04	1.09	56	-0.91	1.39	82	
Laud	0.59	1.38	18	-0.79	1.70	30	
Orle	1.49	1.18	24	-0.51	1.38	39	
Park	0.50	1.26	29	-0.58	1.52	38	
Soda	1.91	1.89	7	-0.54	2.58	9	
Tsuk	0.93	1.95	16	-0.47	1.11	38	
Woll	0.34	1.07	27	-0.36	1.56	45	
All	0.60	1.45	255	-0.42	1.59	389	

Moreover, the uncertainties of OCO-2 and GOSAT retrievals may be another reason for the different performances in these two inversion experiments. We use TCCON retrieval to evaluate the uncertainties of OCO-2 and GOSAT XCO₂ retrievals. For satellite retrievals falling in the model grid box where TCCON sites are located, the closest TCCON retrievals in time or within two hours of satellite overpass time are chosen for comparison. We follow the procedures in Appendix A of Wunch et al. (2011) to do both prior profile and averaging kernel corrections. Table 5 shows the biases and standard deviations grouped globally and at 10 TCCON sites where both OCO-2 and GO-SAT retrievals are available for comparison. The locations of these 10 sites are shown in Figure 2. At most sites except Garm, OCO-2 retrievals have positive biases, while GOSAT retrievals tend to have negative bias except at Bial and Garm sites. It also could be found that the spread of GOSAT

data biases are small, falling in the range of -0.36 to -0.58 ppm at most sites, while the spread of OCO-2 data biases is relatively large, with biases greater than 0.7 ppm at more than half of sites, and in the range of 0.34 to 0.59 ppm only at 3 sites. Overall, GOSAT retrievals (-0.46 ppm) have lower bias than OCO-2 retrievals (0.6 ppm) and the difference between two retrievals is relatively large. It should be noted that due to the limited number of collocated satellite retrievals, the real bias difference might be below 1 ppm. As shown in Table 4, the difference of overall mismatches between GOSAT and OCO-2 data is 0.57 ppm. These indicate that although both OCO-2 and GOSAT products were bias-corrected using TCCON retrievals, the uncertainties of OCO-2 and GOSAT retrievals are still very large, especially for OCO-2 retrieval, resulting in the degraded performance of OCO-2 retrieval, which also suggest that the bias-correction scheme implemented may need to be improved.

5. Summary and Conclusions

In this study, we use both GOSAT and OCO-2 XCO₂ retrievals to constrain terrestrial ecosystem carbon fluxes from Oct 1, 2014 to Dec 31, 2015, using the GEOS-Chem 4D-Var data assimilation system. In addition, one inversion using in situ measurements and another inversion as a baseline, are also conducted. The posterior carbon fluxes estimated from these four inversions at both global and regional scales during Jan 1 to Dec 31, 2015 are shown and discussed. We evaluate the posterior carbon fluxes by comparing the posterior CO₂ mixing ratios against observations from 52 surface flask sites and 13 TCCON sites.

Globally, the terrestrial ecosystem carbon sink (excluding biomass burning emissions) estimated from GOSAT data is stronger than that inferred from OCO-2 data and weaker than that from in situ inversion, but closest to the poor-man inversion estimate. Regionally, in most regions, the land sinks inferred from GOSAT data are also stronger than those from OCO-2 data. Compared with the in situ inversion, GOSAT inversions have weaker sinks in Boreal and most Tropical lands, and much stronger ones in Temperate lands. Compared with the prior fluxes, the inferred land sinks are largely

increased in the temperate regions, and decreased in tropical regions. There are largest changes of the prior fluxes in Northern Temperate regions, followed by Tropical and Southern Temperate regions, and the weakest in boreal regions. The different impact of XCO₂ on the carbon fluxes in different regions is mainly related to the spatial coverage and the amount of XCO₂ data. Generally, a larger amount of XCO₂ data in a region is corresponding to a larger change in the inverted carbon flux in the same region. The different biases of the two XCO₂ retrievals may also give rise to their different inversion performances.

Evaluations of the inversions using CO₂ concentrations from flask measurements and TCCON retrievals show that the simulated CO₂ concentrations with GOSAT posterior fluxes are much closer to the observations than those with OCO-2 estimates. Compared with poor-man inversion, both GOSAT and in situ inversions show evident improvement with the similar reductions of both biases and standard deviations of posterior concentrations, while OCO-2 inversion only displays slight improvement over poor-man inversion. Generally, the posterior biases from GOSAT inversion are significantly reduced in the northern hemisphere and are slightly increased in the southern hemisphere. These suggest that GOSAT data can effectively improve the carbon fluxes estimate in the northern hemisphere.

The GOSAT and OCO-2 XCO₂ retrievals used in this study are bias-corrected products. Nevertheless, there still exists apparent biases and the differences between these two satellites data are obvious. The more reliable constraints on carbon flux call for the further reduction of satellite retrieval errors. These indicate that we should interpret carbon flux inferred from the current satellites XCO₂ retrievals with great cautions in understanding global carbon cycle. It also should be noted that though the OCO-2 XCO₂ retrievals of version b7.3 used in this study perform worse than GOSAT data and in situ measurements in our inversions, one recent study has shown that the newer version of OCO-2 data has a much better performance in constraining carbon flux (Chevallier et al., 2019). With constantly improved retrieval algorithm and bias-correction scheme, more robust estimate of carbon flux

528 from satellite XCO₂ retrievals could be achieved. **Author contributions** 529 FJ and HW designed the research, HW conducted inverse modeling, HW and FJ conducted data anal-530 ysis and wrote the paper, JW, WJ and JC participated in the discussion of the results and provided 531 input on the paper for revision before submission. 532 **Competing interests** 533 The authors declare that they have no conflict of interest. 534 535 Acknowledgements This work is supported by the National Key R&D Program of China (Grant No: 2016YFA0600204), National 536 Natural Science Foundation of China (Grant No: 41571452), and the Fundamental Research Funds for the 537 Central Universities (Grant No: 090414380021). CarbonTracker CT2016 products are provided by NOAA 538 ESRL, Boulder, Colorado, USA from the website at http://carbontracker.noaa.gov. The authors thank all con-539 tributing laboratories for providing in-situ CO₂ observations through ObsPack product obspack co2 1 CAR-540 541 BONTRACKER CT2016 2017-02-06, and TCCON PIs for making XCO2 measurements possible and available to the public. The authors are very grateful to Dr. Feng Deng at the University of Toronto for providing 542 the module for in-situ data inversion, and for his valuable suggestions on running GEOS-Chem adjoint model. 543 The authors would also like to thank two reviewers for their constructive comments which greatly improve the 544 545 manuscript. 546 References 547 548 Andres, R. J., Gregg, J. S., Losey, L., Marland, G. and Boden, T. A.: Monthly, global emissions of carbon 549 dioxide from fossil fuel consumption. Tellus B, 63(3), 309-327, https://doi.org/10.1111/j.1600-550 0889.2011.00530.x, 2011.

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