Inverse Modeling of CO₂ Fluxes Using GOSAT Data and Multi-Year Ground-Based Observations

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Abstract

We present surface CO₂ flux estimates obtained by an inverse modeling analysis from column-averaged dry air mole fractions of CO₂ (XCO₂) observed by the Greenhouse gases Observing SATellite (GOSAT) and ground-based data. Two inversion cases were examined: 1) a decadal inversion using ground-based CO₂ observations by NOAA from 1999 to 2010 to derive CO₂ flux interannual variability, and 2) an inversion using NOAA plus NIES GOSAT XCO₂ data from June 2009 to October 2010. We used single-shot GOSAT data and individual NOAA flask data for the inversions. Our results show differences in estimated fluxes between the NOAA data inversion and the NOAA plus GOSAT data inversion, especially in Northern Eurasia and in Equatorial Africa and America where the ground-based observational sites were sparse. Uncertainty reduction rates of 40%–70% were achieved by inclusion of GOSAT data, compared to the case using just the NOAA data. The inclusion of GOSAT data in the inversion resulted in larger summer sinks in northwest Boreal Eurasia and a smaller summer sink in southeast Boreal Eurasia, with a clear uncertainty reduction in both regions. Adding GOSAT data also led to increase in Tropical African fluxes in boreal winter beyond interannual variability from NOAA data inversions.


1. Introduction

Carbon dioxide (CO₂) is an important greenhouse gas with a large impact on the earth’s climate (e.g., Forster et al. 2007); consequently, an accurate estimate of the global carbon budget is urgently required. Precise measurements of atmospheric CO₂ at fixed ground sites, and from ships, aircraft, and balloons, have been used to elucidate CO₂ variations over the globe in recent decades (e.g., Aoki et al. 2003; GLOBALVIEW-CO₂ 2011; Conway et al. 2012). Inverse modeling approaches using atmospheric transport models with these CO₂ observations are an effective way to estimate carbon fluxes at global and regional scales (e.g. Enting 2002). Recently, satellite observations of CO₂ or column-averaged dry air mole fraction of CO₂ (XCO₂) have received much attention because of their nearly global coverage and high temporal and spatial resolution (e.g., Buchwitz et al. 2005; Kulawik et al. 2010; Foucer et al. 2011; Yoshida et al. 2011; Crisp et al. 2012; O’Dell et al. 2012), and satellite-retrieved CO₂ data are now used together with ground-based observations in inverse modeling studies for regional carbon flux estimations (e.g., Engelen and McNelly 2005; Chevallier et al. 2009; Nassar et al. 2011; Takagi et al. 2011; Maksyutov et al. 2012).

The Thermal And Near-infrared Sensor for carbon Observation—Fourier Transform Spectrometer (TANSO–FTS) onboard the Greenhouse gases Observing SATellite (GOSAT) has provided nearly global distributions of XCO₂ from short-wavelength infrared (SWIR) spectra since 2009 (Kuze et al. 2009; Yokota et al. 2009). The GOSAT XCO₂ data are expected to contribute accurate estimates of the global carbon budget and to reduce the estimated flux uncertainty because of their wide spatial coverage and high temporal resolution. Here we conduct a multi-year inversion with ground-based CO₂ data and a one-year inversion with ground-based data plus GOSAT XCO₂ data, and compare their results to assess estimated fluxes using the interannual variability (IAV) of fluxes estimated from decadal ground-based data, and assess if GOSAT data has potential to contribute new findings to carbon budget analysis.

2. Data and method

Flask-sampled atmospheric CO₂ data (1999–2010) collected at 95 sites from the Cooperative Air Sampling Network coordinated by the Global Monitoring Division of the Earth System Research Laboratory, the National Oceanic and Atmospheric Administration (NOAA) (hereafter called “NOAA data”) (Conway et al. 2012) were used (see NOAA site location in Fig. 1). Data uncertainty assigned to the NOAA data was monthly standard deviations taken from GLOBALVIEW-CO₂ (2011). Following Gurney et al. (2004), the minimum uncertainty was defined as 0.25 ppm. For satellite observations, we used the National Institute for Environmental Studies (NIES) GOSAT SWIR XCO₂ Level 2 product (version 2.00 and 2.10, available at https://data.gosat.nies.go.jp/) over the period from June 2009 to October 2010. The GOSAT data used here were subjected to a standard filtering and screening applied for general distribution. In the version we used, its bias and standard deviation (~1.20 ± 1.96 ppm) (Yoshida et al. 2013) are lower than the previous version (V1.xx) of the product relative to the Total Carbon Column Observing Network (TCCON) observations (Wunch et al. 2011, version GGG2009) (Morino et al. 2011). The present study differs from previous inversion works by Takagi et al. (2011) and Maksyutov et al. (2012) which used monthly averaged GOSAT data by NIES aggregated on 5° × 5° grids and monthly averaged GLOBALVIEW data. We used single-shot GOSAT data and individual NOAA flask data for the inversions. For single-shot GOSAT data, the uncertainty assigned to each single shot was 2.25 ppm, which was estimated as the sum of data uncertainty (2.00 ppm, taken from the standard deviation of 1.96 ppm against TCCON observations) and model uncertainty of 0.25 ppm. The number of GOSAT XCO₂ data per month ranges...
from 4264 to 9264 from the target period of June 2009 to October 2010.

Our inverse modeling system consists of a NIES off-line atmospheric transport model (NIES-TM) version 08.1 (Belikov et al. 2013) and a fixed-lag Kalman smoother (Saeki et al. 2013). Monthly regional carbon fluxes are estimated for 64 regions (42 land and 22 ocean regions, shown in Fig. 1). The NIES-TM was implemented with $2.5^\circ \times 2.5^\circ$ horizontal resolution and 32 vertical levels in a hybrid sigma-isentropic ($\sigma - \theta$) coordinate system. We obtained carbon flux $s$ by minimizing a cost function, $J$ defined as below:

$$J = \frac{1}{2} \left( (z - Hs)^\top R^{-1} (z - Hs) + (s - s_0)^\top Q^{-1} (s - s_0) \right)$$

(1)

where $z$ is difference between model predictions and observations, $H$ is an observation operator that maps surface fluxes in the model space to the measurement space, $s_0$ is the vector of the a priori flux, and $R$ and $Q$ are error variance–covariance matrices for the model-data mismatch and a priori flux estimates, respectively. Off-diagonal elements of the error covariance matrices $R$ and $Q$ were set to zero under the assumption that the data or a priori fluxes in different areas were uncorrelated. In our optimization, before moving to the next assimilation window of the Kalman smoother, the final estimate of carbon fluxes $s$ at the current assimilation window was multiplied by the CO$_2$ concentration fields of dropped response functions that were no longer being used for the optimization, and then propagated into the forward model prediction for the next assimilation step (Saeki et al. 2013). Since the satellite-observed XCO$_2$ represents a weighted average over an entire atmospheric column, simulated CO$_2$ profiles were weighted by using averaging kernels in the GOSAT data products to obtain a GOSAT-equivalent XCO$_2$ quantity. The a priori flux dataset used to predict background CO$_2$ concentrations was composed of four datasets listed Table 1. The flux datasets are available for the period from 2000 to 2010 at $1^\circ \times 1^\circ$ spatial resolution. For the year 1999 simulation for spin-up, the 2000 fluxes were used. Monthly a priori flux uncertainties for 64 land and ocean regions were derived from the 2000–2010 VISIT and OTTM products, respectively.

Two inversion cases were conducted using (1) 1999–2010 NOAA data and (2) NOAA plus GOSAT data for the period from June 2009 to October 2010. The forward model simulation was initialized on 1 January 1999 with the zonal average CO$_2$ concentration based on a three-dimensional CO$_2$ climatology, the Gap-Filled and Ensemble Climatology Mean (Saito, R. et al. 2011). The lag length of the fixed-lag Kalman smoother was set to 4 months. We assume two global offsets for NOAA data and for GOSAT data as unknown parameters at the first step of our inversions. After the first 4-month run, the estimated global offset value was treated as a known value. Then, the simulation was recalculated from the beginning using the initial concentration field plus the estimated global offsets; these offsets were set to be constant during the subsequent optimization steps. The global offsets were estimated 0.36 ppm for NOAA data and $-0.11$ ppm for GOSAT data. The data uncertainty of NOAA data was scaled up by 1.3 to obtain an average chi-squared ($\chi^2$) value (see Supplement for definition) of 1.01 over the inversion period 1999–2010. Observational data that showed large model–data mismatch were given a large data uncertainty to effectively exclude their effect. The rejection criteria were model–data mismatch greater than 3 times their uncertainty for NOAA data, and 1.5 times for GOSAT data. The rates of rejection are 4.5% and 21% for GOSAT single-shot data (the total number is 289737) and NOAA flask data (10593) from June 2009 to May 2010 with 4-month window. Under these conditions, the NOAA plus GOSAT inversion resulted in $\chi^2 \approx 1$ for the target period.

3. Results and discussion

To illustrate the influence of adding GOSAT XCO$_2$ data to the ground-based NOAA data, differences in the estimated carbon fluxes between the NOAA plus GOSAT data inversion and the NOAA data only inversion in July 2009 and January 2010 are presented in Fig. 2, and Table 2 lists carbon flux for selected regions from this study and published studies. The rate of uncertainty reduction (UR) in percent can be used as a measure of the contribution of GOSAT data to reducing uncertainty in estimated fluxes (Fig. S2). Overall statistics shows a forward simulation with the inverted fluxes shows better performance than a free-run simulation with a priori fluxes only, though slightly (Fig. S3).

Differences in estimated fluxes between NOAA data and NOAA plus GOSAT data inversions are small for regions where NOAA data constrain the fluxes well, such as western North America (Regions 5, 7) and Western Europe (Regions 39, 40, 41) (Fig. 2). Their associated uncertainty reduction rates are also small (Fig. S2), and the estimated flux from the NOAA plus GOSAT data is within the IAV of the fluxes from the NOAA data. For example, the estimated monthly flux in Region 7 (Fig. 3a) from NOAA plus GOSAT data is within NOAA climatological fluxes derived from the 1999–2010 NOAA-data inversion. Also, the flux difference and the uncertainty reduction rates are quite small in northern Tropical Africa (Regions 19, 20) where GOSAT provides plenty of XCO$_2$ data throughout the year (Fig. S1) because the assigned a priori flux uncertainties are very small in these desert areas (the maximum uncertainty through the year is 0.4 and 0.02

Table 1. Summary of a priori fluxes used for the inverse modeling.

<table>
<thead>
<tr>
<th>Flux Type</th>
<th>Database Name</th>
<th>Time resolution</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anthropogenic CO$_2$ emissions (fossil fuel CO$_2$ emissions plus cement manufacturing)</td>
<td>ODIAC (Open source Data Inventory of Anthropogenic CO$_2$ emission)</td>
<td>Monthly</td>
<td>An updated version of Oda and Maksyutov, 2011</td>
</tr>
<tr>
<td>Net ecosystem exchange</td>
<td>VISIT (Vegetation Integrative Simulator for Trace gases)</td>
<td>Daily</td>
<td>Ito, 2010</td>
</tr>
<tr>
<td>Biomass burning</td>
<td>GFED (Global Fire Emissions Database) version 3.1</td>
<td>Monthly</td>
<td>van der Werf et al., 2010</td>
</tr>
<tr>
<td>Air–sea CO$_2$ exchange</td>
<td>OTTM (the Offline ocean Tracer Transport Model)</td>
<td>Monthly</td>
<td>Valsala and Maksyutov, 2010</td>
</tr>
</tbody>
</table>
GtC/yr for Region 19 and 20, respectively) and there is no scope for flux changes. Most oceanic regions generally show little change compared with changes over land because the magnitudes of oceanic fluxes are relatively small (about ±0.5 gC m$^{-2}$ day$^{-1}$ (Fig. 2)).

The differences in the estimated fluxes in July are considerable in Boreal Eurasia (Regions 25–28, 42) (Fig. 2; Table 2) where a particularly high uncertainty reduction rate of 70% is indicated (Fig. S2). Compared to Maksyutov et al. (2012) who used GOSAT data averaged over a 5° × 5° grid cell on a monthly time scale, our direct use of GOSAT single-shot data resulted in 10%−20% larger uncertainty reduction rates for these regions. This area contains no NOAA observational sites, while GOSAT provided over a wide area of Boreal Eurasia in boreal summer (Fig. S1). GOSAT observations have less impact on estimated Boreal Eurasian fluxes in winter because observations are few, due to large solar zenith angles (Yoshida et al. 2011), as illustrated in Fig. S1.

The estimated monthly fluxes from June 2009 to May 2010 for southeast Boreal Eurasia (Region 26) and northwest Boreal Eurasia (Region 27) are shown in Figs. 3b and 3c, respectively, as well as the statistics of the NOAA inversion results from 1999 to 2010. We found GOSAT data weaken the boreal summer fluxes for southeast Boreal Eurasia (Region 26) and strengthen the fluxes for northwest Boreal Eurasia (Region 27), respectively, and significantly reduce the uncertainty. Changes in the estimated flux in August with GOSAT data are most notable, giving positive flux

| Table 2. Comparison of carbon fluxes [GtC/yr/region] for selected regions from this study and published studies. |
|-------------------------------------------------|-------------------------------------------------|-------------------------------------------------|---------------------------------|---------------------------------|
| This study                                      | Maksyutov et al., 2012a, b                      | Other estimates                                 |
| Fluxes                                          | A priori fluxes                                 | A priori fluxes                                 | Estimated fluxes                | Estimated fluxes                |
| Region                                          | (NOAA data)                                     | (NOAA plus GOSAT data)                          | (NOAA data)                     | (NOAA plus GOSAT data)          |
| North Africa (Regions 17–20)                    | 0.24±1.88                                        | 0.30±1.88                                        | 2.23±0.98                       | 1.10±1.53                       |
| Boreal Eurasia (Regions 25–28)                  | −0.11±2.38                                      | −0.31±1.28                                      | −0.47±0.88                      | −0.52±1.11                      |
| South Asia (Region 30)                          | −0.0045±1.00                                    | 0.0062±1.00                                     | −0.23±0.81                      | −0.48±0.58                      |
| East Asia (Region 32)                           | −0.16±3.01                                      | −0.12±3.01                                      | 0.067±0.48                      | −0.37±0.20                      |

aBiomass burning emissions are included in the land fluxes, but fossil fuel emissions are not.
bData was downloaded from GOSAT GUIG (https://data.gosat.nies.go.jp/) (last access: 25 February 2013).
cEast Asia in Piao et al. covers area of 12 × 10^6 km^2 while Region 32 in this study is 7.41 × 10^6 km^2.
for Region 26 and a negative flux for Region 27. These changes are not within the decadal IA V of the estimated fluxes. This tendency is consistent with the finding that adding Siberian surface and aircraft observations weakens the summer sink seen in the NOAA dataset over southeast Boreal Eurasia (Region 26) (Saeki et al. 2013) (Table 2). The year 2009 is close to the climatological mean over Russia since the 1970s (Dolman et al. 2012), and flux changes over Boreal Eurasia are generally within the decadal flux variability, but when the GOSAT observations are taken into account in estimating Siberian flux, the confidence level of the Siberian regional carbon estimate increases.

The impact of the use of GOSAT data also can be seen over West and South Asia, such as southwest and southeast Temperate Asia (Regions 29 and 30, respectively), with uncertainty reduction rates in the range of 30%−60%, and a particularly high reduction rate in October 2009 (figure not shown) when GOSAT provides XCO₂ data over most of these areas. For Region 29, flux changes can be seen in the northern part of the area (Fig. S2), and the maximum reduction in uncertainty reaches about 60% in October, which is consistent with estimates from previous studies (Takagi et al. 2011; Maksyutov et al. 2012). In spite of the large reduction in uncertainty in Region 29, the flux change obtained by including GOSAT data is small and within decadal IA V fluxes. In Region 30 (mainly India), where GOSAT coverage is good in boreal winter (Fig. S1), the GOSAT data generally brought flux change towards negative (Fig. 2) and outside of the decadal IA V with significance (Fig. S1), and the differences in the estimated fluxes over Tropical Africa (Region 17). The inclusion of GOSAT data gives fluxes from November to February 2010 that are higher than the past 10 years’ fluxes, which is also stronger source than a previous estimate by Baker et al. (2006) (Table 2). The Inter-Tropical Convergence Zone (ITCZ) is situated over Tropical Africa during this season, and strong convective activity associated with the ITCZ may make it easier for GOSAT to observe surface flux changes, although ITCZ is accompanied by convective cloud. Tropical Africa is one of the regions where satellite observations were expected to reduce uncertainty (Chevallier et al. 2009; Feng et al. 2009), and multi-year analysis using GOSAT data might be valuable in quantifying the Tropical African flux.

4. Conclusion and outlook

We derived regional carbon fluxes using both NOAA data alone and NOAA together with GOSAT data (June 2009 to October 2010) by using the NIES atmospheric transport model and a fixed-lag Kalman smoother, and compared the results with (I)GOSAT (1999−2010) inverted fluxes with NOAA data. The results indicated that NOAA data were sufficient to constrain the fluxes in North America and Western Europe, and the inclusion of GOSAT data resulted in little change in the estimated fluxes. The benefit of GOSAT data was clearly seen over Boreal Eurasia and parts of North America in boreal summer and over Equatorial Africa and America in boreal winter. Regional flux uncertainty reduction rates compared with the NOAA data inversion reached 40%−70%, which is higher than in previous publications due to use of GOSAT observations without aggregation. We used 17 months of GOSAT data. Extension of the GOSAT L2 product time series is in progress at NIES, and multi-year flux estimation will become available, which may reveal more clearly
the benefit of GOSAT observations. Bias correction of GOSAT L2 data might be one of the aims of future work. Though this study relies more on the NOAA data than the GOSAT data (i.e. minimum uncertainties of 0.25 and 2.25, respectively), ongoing studies on the retrieval method and validation analysis of the improved GOSAT data may enable more reliable surface flux estimations from GOSAT data.

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Supplement

Supplement presents definitions of chi-square value and the estimated fluxes uncertainty, global distributions of monthly averaged GOSAT-derived XCO₂ (Fig. S1), uncertainty reduction rates (Fig. S2), and a statistical comparison between a free run and a run with the inverted fluxes (Fig. S3).

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