Comparing simulated atmospheric carbon dioxide concentration with GOSAT retrievals

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Abstract Satellite observations of atmospheric carbon dioxide (CO₂) provide a useful way to improve the understanding of global carbon cycling. In this paper, we present a comparison between simulated CO₂ concentrations from an inversion model of the CarbonTracker Data Assimilation System (CTDAS) and satellite-based CO₂ measurements of column-averaged dry air mole fraction (denoted XCO₂) derived from version 3.3 Atmospheric CO₂ Observations from Space retrievals of the Greenhouse Gases Observing SATellite (ACOS–GOSAT) L2 data products. We examine the differences of CTDAS and GOSAT to provide important guidance for the further investigation of CTDAS in order to quantify the corresponding flux estimates with satellite-based CO₂ observations. We find that the mean point-by-point difference (CTDAS–GOSAT) between CTDAS and GOSAT XCO₂ is -0.11 ± 1.81 ppm, with a high agreement (correlation $r = 0.77$, $P < 0.05$) over the studied period. The latitudinal zonal variations of CTDAS and GOSAT are in general agreement with clear seasonal fluctuations. The major

exception occurs in the zonal band of 0°–15°N where the difference is approximately 4 ppm, indicating that large uncertainty may exist in the assimilated CO₂ for the low-latitude region of the Northern Hemisphere (NH). Additionally, we find that the hemispherical/continental differences between CTDAS and GOSAT are typically less than 1 ppm, but obvious discrepancies occur in different hemispheres/continents, with high consistency (point-by-point correlation $r = 0.79$, $P < 0.05$) in the NH and a weak correlation (point-by-point correlation $r = 0.65$, $P < 0.05$) in the Southern Hemisphere. Overall, the difference of CTDAS and GOSAT is small, and the comparison of CTDAS and GOSAT will further instruct the inverse modeling of CO₂ fluxes using GOSAT.

Keywords CTDAS model · Satellite-based CO₂ concentration · GOSAT · Comparison · Inversion method

1 Introduction

Accurate quantification of biosphere fluxes of CO₂ is critical to understanding global and regional carbon cycles [1, 2]. The atmospheric inversion method provides an effective way to quantify the biosphere CO₂ concentration/flux at the full-coverage spatial resolutions [3–7]. This approach derives the CO₂ concentrations and fluxes jointly from an atmospheric transport model and data assimilation technique. Unlike ecosystem modeling [8–15], the inverted method uses the atmospheric CO₂ transport process mechanism to describe the CO₂ spatiotemporal variations and uses the time-dependent Bayesian synthesis method to optimize the CO₂ concentrations and fluxes. This is advantageous for CO₂ estimation because the

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concentrations and fluxes can be constrained well by the observations in the inversion model. However, because of the sparseness of the existing CO₂ mixing ratio observation sites, the inversion estimate of CO₂ concentrations and CO₂ source and sink information remain unclear [16–19].

Satellite-based CO₂ observations of column-averaged dry air mole fraction (XCO₂) offer a new insight into the pattern of CO₂ mixing ratios and provide an additional constraint on the estimated CO₂ concentrations and fluxes of the atmospheric inversion method [16, 19–22]. These satellite-based measurements (e.g., GOSAT [23], AIRS [24], SCIAMACHY [25] and IASI [26]) allow for the quantification of large-scale temporal, spatial and seasonal variations in CO₂. As the first-dedicated greenhouse gas sensor [19, 23], GOSAT has been particularly useful for improving estimates of CO₂ concentrations and decreased uncertainties of CO₂ sources and sinks by providing further constraints on the inversion method [26–28], since it was specifically designed for monitoring high-precision observations of CO₂ concentrations with sensitivity in the lower troposphere [23, 29]. However, errors in GOSAT observations and models still need to be identified and minimized before these satellite-based measurements are assimilated into the inversion model, as they could lead to additional uncertainties of the inferred CO₂ concentrations and fluxes and result in misinterpretation of the global and regional carbon cycles. In this context, we present a comparison between GOSAT XCO₂ retrieved from version 3.3 Atmospheric CO₂ Observations from Space retrievals of the Greenhouse Gases Observing SATellite (ACOS–GOSAT) L2 data products [30–32] with the CarbonTracker Data Assimilation System (CTDAS) [6, 33] CO₂ concentrations during April 2009–December 2010. We examined the differences of CTDAS and GOSAT to provide important guidance for the further investigation of CTDAS in order to quantify the corresponding flux estimates with satellite-based CO₂ observations.

2 Methods and data

2.1 GOSAT XCO₂ retrievals

We use the GOSAT XCO₂ L2 data products (Version 3.3) from the NASA Atmospheric CO₂ Observations from Space (ACOS3.3) XCO₂ retrievals [30–32] to compare with our CTDAS XCO₂ retrievals during April 2009–December 2010. These ACOS3.3 XCO₂ retrievals have already been evaluated by comparison with ground-based measurements of XCO₂ from Total Column Observing Network (TCCON) stations [30, 31] and have been successfully employed in many previous works [32, 34–36]. The ACOS3.3 XCO₂ retrievals were downloaded from

NASA Goddard Earth Sciences Data (<http://disc.sci.gsfc.nasa.gov/acdisc/documentation/ACOS.shtml>) for this study. Compared to the ACOS2.9, ACOS3.3 XCO₂ retrievals have changed their CO₂ absorption cross sections to 2.06 micro-bands, which are systematically ~1 % lower than the XCO₂ retrievals using 1.61 micro-bands, resulting in large differences in measurement values. Note that before the ACOS3.3 XCO₂ were used in this study, we applied an updated screening criteria to filter out the ACOS3.3 XCO₂ measurements and corrected their biases according to the reference of “ACOS Level 2 Standard Product Data User’s Guide, version 3.3” (available from <http://disc.sci.gsfc.nasa.gov/datareleases/acos-version-3.3>).

2.2 CTDAS model

CTDAS (<http://carbontracker.eu/ctdas/>) [6, 33] was developed to estimate the global CO₂ surface fluxes and atmospheric CO₂ concentration distribution with high accuracy and precision [4, 6, 37–41]. First, the system forecasted the atmospheric CO₂ concentrations using the transport model TM5 [42] and then optimized these modeled CO₂ concentrations and flux fields using the data assimilation technique in CTDAS. In this study, we ran CTDAS using weekly resolution and a 5-week lag window to retrieve the volume mixing ratio of CO₂ (CTDAS XCO₂) sampled at GOSAT locations and times, based on method of Rodgers and Connor [43]. The CTDAS simulation spanned the period from 2008 to 2010, but the period from January 2008 to March 2009 was used as a spin-up period to initialize the model and was therefore excluded from our analysis. The driving meteorological data in CTDAS were from the European Centre for Medium-Range Weather Forecasts (ECMWF, <http://www.ecmwf.int/research/ifsdocs/CY28r1/index.html>), and CTDAS was forced by four prior surface fluxes: (1) the first guess biosphere flux extracted from the Carnegie–Ames–Stanford Approach (CASA, <http://geo.arc.nasa.gov/sge/casa/index4.html>) [44]; (2) the fossil fuel emissions integrated from the Carbon Dioxide Information and Analysis Center (CDIAC) [45] and the Emission Database for Global Atmospheric Research (EDGAR) database [46]; (3) the biomass burning emissions obtained from Global Fire Emission Database version 2 (GFED2, <http://ess1.ess.uci.edu/jranders/data/GFED2>); and (4) the prior ocean fluxes derived from air–sea partial pressure difference [47]. The CO₂ measurements at the surface were assimilated in this system from the National Oceanic and Atmospheric Administration’s Earth System Research Laboratory (NOAA-ESRL, <http://www.esrl.noaa.gov/gmd/ccgg/obspack/>). The simulated 4-D (x, y, z, t) CO₂ concentration fields contain 25 vertical layers with a global horizontal resolution of 6° × 4°.

3 Results and discussion

3.1 Comparison between CTDAS and GOSAT

Here, we compare the estimated CTDAS XCO_2 with the observed GOSAT XCO_2 retrievals. Our CTDAS XCO_2 was calculated based on the GOSAT averaging kernel and prior profile. Following the method of Rodgers et al. [43], the retrieved XCO_2 of CTDAS can be expressed as:

$$XCO_2 = h^T X_a + h^T A(X_h - X_a), \quad (1)$$

where h^T presents the transpose of the GOSAT pressure-weighting function; X_a is the GOSAT's prior profile; A is the averaging kernel matrix of GOSAT; and X_h is the modeled vertical CO_2 concentration profile interpolated at the GOSAT's vertical layers.

Figure 1 shows the comparison between CTDAS and GOSAT XCO_2 for each season during the period of April 2009–December 2010. The spatial distributions of CTDAS and GOSAT XCO_2 change seasonally, all with the highest CO_2 concentration in spring and the lowest CO_2 in summer. These global seasonal variations are reasonable and agree with many previously published results [19, 48]. For the whole study period, there is general agreement between CTDAS and GOSAT with point-by-point correlation of 0.77 ($P < 0.05$). The mean point-by-point difference (CTDAS – GOSAT) is -0.11 ± 1.81 ppm, seasonally varying from -0.01 to -0.66 ppm, with the largest difference in winter (-0.66 ± 1.72 ppm) and the smallest bias in autumn (-0.01 ± 1.71 ppm). This model-observation bias

is consistent with the previous results reported by Peters et al. [33] that the CTDAS model can accurately simulate CO_2 concentrations, in which CTDAS is on average within 0.5 ± 0.9 ppm bias compared with the independent column-averaged CO_2 concentrations measured by Fourier transform spectrometer (FTS) at the site levels.

We find that the mean standard deviation of GOSAT XCO_2 is relatively large (~ 1.99 ppm in CTDAS vs. ~ 2.82 ppm in GOSAT), suggesting a large variation in the satellite-based XCO_2 , while the modeled column mix fraction retrievals show comparatively unscattered distributions. This is partly due to the effects of heterogeneous sources and complicated climate conditions in the atmosphere, leading to substantial variance of the spatial patterns of atmospheric CO_2 . This variability is hard to be comprehensively reproduced by modeled XCO_2 , as only an average estimate is produced (unscattered standard deviation), but well captured by GOSAT with high spread, corresponding to the true atmospheric CO_2 variance. On the other hand, perturbation of clouds and aerosols to satellite-based XCO_2 could also introduce additional observed scatters into GOSAT measurements and extend the range of standard deviation [20, 30].

Latitudinal comparisons between CTDAS and GOSAT XCO_2 retrievals are presented in Fig. 2 with 5° zonal averages between $40^\circ S$ and $60^\circ N$. Note that the bias and correlation coefficient given here are very different from the values in Fig. 1. The values in Fig. 1 and their associated texts are calculated point-by-point, while the values in Fig. 2 and their associated texts are calculated zone-by-zone by

Fig. 1 Comparison of GOSAT XCO_2 with CTDAS XCO_2 calculated from CTDAS based on GOSAT averaging kernel. Each seasonal column-averaged CO_2 concentrations are shown for (a) CTDAS XCO_2 , (b) GOSAT XCO_2 and (c) the difference between CTDAS and GOSAT (difference = CTDAS – GOSAT)

Fig. 2 (a) Latitudinal zonal means and (b) zonal difference as well as their standard deviation between 40°S and 60°N in 5° bins for CTDAS and GOSAT XCO₂ retrievals are presented during April 2009–December 2010. Note that the bias and correlation coefficient given here are very different from the values in Fig. 1. The values in Fig. 1 and their associated texts are calculated through point-by-point way, while the values in Fig. 2 and their associated texts are calculated through latitudinal zone-by-zone way

latitude. Overall, there is a strong correlation coefficient (latitude zone-by-zone correlation $r = 0.79$ $P < 0.05$, Bias = -0.38 ± 0.64 ppm) between the model and observed zonal latitudinal gradients with a clear seasonal fluctuation. In spring, the latitudinal gradients show higher correlation (latitude zone-by-zone correlation $r = 0.92$ $P < 0.05$, Bias = -0.68 ± 0.93 ppm) and lower XCO₂ in Southern Hemisphere (SH) than the northern latitudes, which is consistent with the effect of the seasonal cycle on inter-hemisphere CO₂ concentration [34]. The zonal mean hemispheric gradients in summer also have high correlation (latitude zone-by-zone correlation $r = 0.95$ $P < 0.05$, Bias = -0.01 ± 0.53 ppm) between CTDAS and GOSAT XCO₂ retrievals and show a pronounced CO₂ decrease in the northern latitudes. In autumn, CTDAS zonal gradient has a relatively poor correlation (latitude zone-by-zone correlation $r = 0.66$ $P < 0.05$, Bias = -0.23 ± 0.54 ppm) with observed values. This is inconsistent with the previous findings that comparisons between modeled and observational CO₂ seasonal variations show accurate timing in autumn, but a large mismatch summer at the surface site-level [49–51]. This discrepancy is likely due to a shift in the timing of summer XCO₂, as the CO₂ column-averaged dry air mole fraction of CTDAS and GOSAT lagged in the lowest annual cycle causing the stronger summer vegetation photosynthesis uptake of CO₂ to occur in July–October, rather than June–August. This resulted in a partial mismatch of the vegetation carbon uptake in the autumn season. For winter, despite poor GOSAT data coverage in the high northern latitude due to persistent cloud and solar zenith angle restriction [34], the XCO₂ shows a relatively high latitudinal zone-by-zone correlation ($r = 0.80$ $P < 0.05$, Bias = -0.51 ± 1.04 ppm) but much lower global point-by-point correlation ($r = 0.59$ $P < 0.05$, Bias = -0.66 ± 1.72 ppm) between GOSAT and CTDAS.

Over the regions of latitude bands of 0°–15°N, we found differences between the CTDAS XCO₂ and GOSAT XCO₂

of up to ~ 4 ppm during April 2009 to December 2010, indicating that large uncertainty potentially exists in the assimilated CO₂ for the low-latitude region of the NH. This uncertainty in our estimation can be partly explained by the lack of the available observation sites in the tropical and subtropical areas of the NH. A greater amount of human activities and local carbon emissions over this region also contribute to this uncertainty, further increasing the bias between the simulated and observed values [5, 52–54]. In addition, a large standard deviation (~ 2.0 ppm) to the simulated-minus-observed difference was found in the Northern middle- to high latitude zones (50°–60°N), mainly due to solar zenith angle restrictions and cloud contamination, which cause large errors in GOSAT XCO₂ [20, 34].

Figure 3 shows the time series of XCO₂ from CTDAS and GOSAT, for NH and SH in (a–b) as well as seven different continents in (c–i). As the effect of the natural CO₂ sources and human activities are more variable on the land, the hemispheric variations of both the CTDAS and GOSAT XCO₂ are significantly different, with higher (lower) XCO₂ concentrations and more (less) seasonal fluctuation over the NH (SH) land [20, 48]. We found that the seasonal cycle agrees well between CTDAS and GOSAT for the NH (point-by-point correlation $r = 0.79$ $P < 0.05$) and the SH (point-by-point correlation $r = 0.65$ $P < 0.05$), with bias of -0.04 ± 1.96 and -0.25 ± 1.45 ppm, respectively. This is inconsistent with Cogan et al. [20] and Qu et al. [48] that show a larger bias in the NH. This discrepancy is partly due to the compensation effect of a positive bias (overestimate) in the lowest peak and a negative bias (underestimate) in the highest peak of CTDAS XCO₂ time series, leading to a small mean bias in the NH, but still with a large amount of scatter (e.g., standard deviation of ~ 1.96 ppm) in simulated XCO₂.

The time series of XCO₂ shows variations in different months and continents (Fig. 3). In Europe and North

Fig. 3 Comparisons of CTDAS and GOSAT XCO₂ for Northern/Southern Hemisphere in (a–b) and for seven continents in (c–i) outlined on the map between April 2009 and December 2010. The error bars represent the standard deviation of the CTDAS and GOSAT data, respectively. Note that the bias and correlation coefficient given here are calculated through point-by-point way

America, CTDAS and GOSAT XCO₂ show strong agreement (point-by-point correlation $r = 0.80$, $P < 0.05$, $r = 0.81$, $P < 0.05$, respectively) in the magnitude and phase of XCO₂ with many CO₂ sources in this region [19]. Asia, which contains a large area of desert (GOSAT XCO₂ observed with high gain model) and high CO₂ emissions, has good consistency with the mean XCO₂ bias of 0.04 ppm and point-by-point correlation coefficient of 0.80 in time series, but a slightly high standard deviation (~ 2.08 ppm). In Africa, we found consistency between observed and modeled XCO₂ in the amplitude of the seasonal cycle (point-by-point correlation $r = 0.76$, $P < 0.05$). In the Northern Hemispheric continents, the model can capture over 80 % of the observed variability, whereas only 50 %–60 % of the observed variability can be captured in South America and Australia, which may attribute to weakness in the model. As expected, we see a

low positive correlation in Oceania between GOSAT and CTDAS (point-by-point correlation $r = 0.56$, $P < 0.05$), with the magnitude of XCO₂ seasonal cycle slightly overestimating the XCO₂ in model.

3.2 Robustness of CTDAS

CTDAS provides a useful way to estimate CO₂ concentrations and fluxes by integrating the atmospheric transport model, the data assimilation technique, prior fluxes and CO₂ observations. While incorporating these techniques and data can be powerful to improve the understanding of the CO₂ sources and sinks, it also implies that the assimilated CO₂ distribution can be influenced by introduced sources of uncertainty in the CO₂ assimilation system. Such uncertainty includes uncertainty in the prior fluxes, biases in the observations and errors in the atmospheric

transport model. Our estimates of CO₂ are sensitive to these uncertainties, especially for the systematic errors in the atmospheric transport model [6, 17]. Any mis-specification in the atmospheric transport model, such as insufficient spatiotemporal resolutions, incorrect atmospheric vertical transport and poor driving meteorological data, could introduce large uncertainty in estimates. Another disadvantage to the assimilated CO₂ distribution is that the uncertainty associated with the atmospheric transport model is not quantified, which is an important limitation and has been identified as a shortcoming in the current CO₂ assimilation system [17, 34, 55]. All of these uncertainties in CTDAS could result in a fraction of the differences between CTDAS and GOSAT.

4 Conclusion

We compared simulated XCO₂ with the satellite-based measurements to quantify the differences between CTDAS and GOSAT. The spatial and temporal patterns of CTDAS show a high agreement (point-by-point correlation $r = 0.77$, $P < 0.05$) with GOSAT. The mean point-by-point difference (CTDAS – GOSAT) is -0.11 ± 1.81 ppm, seasonally varying from -0.01 to -0.66 ppm, with the largest difference in winter (-0.66 ± 1.72) ppm and the smallest bias in autumn (-0.01 ± 1.71) ppm. The largest latitudinal zonal bias was found in the band of 0° – 15° N (~ 4 ppm), partly due to impact of sparse observations and strong influence of human activities and local carbon emissions over this region. We additionally found that the hemispherical and continental differences between CTDAS and GOSAT are typically less than 1 ppm, reproducing most of the observed variability for Northern and Southern Hemispheres. However, differences occur in the amplitude of seasonal cycle over different hemispheres, with high consistency in the NH (point-by-point correlation $r = 0.79$, $P < 0.05$) and a weak correlation in the SH (point-by-point correlation $r = 0.65$, $P < 0.05$). Overall, the difference of CTDAS and GOSAT is generally small and this comparison will further instruct the inverse modeling of CO₂ fluxes using GOSAT.

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Conflict of interest The authors declare that they have no conflict of interest.

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