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Spatio-Temporal Consistency Evaluation of XCO₂ Retrievals from GOSAT and OCO-2 Based on TCCON and Model Data for Joint Utilization in Carbon Cycle Research

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Abstract: The global carbon cycle research requires precise and sufficient observations of the column-averaged dry-air mole fraction of CO₂ (XCO₂) in addition to conventional surface mole fraction observations. In addition, assessing the consistency of multi-satellite data are crucial for joint utilization to better infer information about CO₂ sources and sinks. In this work, we evaluate the consistency of long-term XCO₂ retrievals from the Greenhouse Gases Observing Satellite (GOSAT), Orbiting Carbon Observatory 2 (OCO-2) in comparison with Total Carbon Column Observing Network (TCCON) and the 3D model of CO₂ mole fractions data from CarbonTracker 2017 (CT2017). We create a consistent joint dataset and compare it with the long-term model data to assess their abilities to characterize the carbon cycle climate. The results show that, although slight increasing differences are found between the GOSAT and TCCON XCO₂ in the northern temperate latitudes, the GOSAT and OCO-2 XCO₂ retrievals agree well in general, with a mean bias $\pm$ standard deviation of differences of 0.21 ± 1.3 ppm. The differences are almost within ± 2 ppm and are independent of time, indicating that they are well calibrated. The differences between OCO-2 and CT2017 XCO₂ are much larger than those between GOSAT and CT XCO₂, which can be attributed to the significantly different spatial representatives of OCO-2 and the CT-transport model 5 (TM5). The time series of the combined OCO-2/GOSAT dataset and the modeled XCO₂ agree well, and both can characterize significantly increasing atmospheric CO₂ under the impact of a large El Niño during 2015 and 2016. The trend calculated from the dataset using the seasonal Kendall (S-K) method indicates that atmospheric CO₂ is increasing by 2–2.6 ppm per year.

Keywords: OCO-2; GOSAT; TCCON; carbon dioxide; CarbonTracker; joint dataset

1. Introduction

The atmospheric carbon dioxide (CO₂) concentration has increased by 40% since pre-industrial times, which has mainly been caused by emissions from fossil fuels and land use changes [1]. However, only less than half of the anthropogenic CO₂ emissions has remained airborne and has become the main driver of climate change, and the remainder is currently being absorbed by the oceans and taken up by the terrestrial biosphere [1,2]. However, these processes are far from well understood. Obtaining a better understanding of the CO₂ sources and sinks to further improve our ability to predict and mitigate climate change requires precise observations with finer spatio-temporal resolutions [3].

There are two common approaches to estimating CO₂ sources and sinks on land: bottom-up and top-down methods. However, both methods have limitations, and large uncertainties still exist.

The bottom-up methods, such as biosphere models and ocean biogeochemistry models, simulate the process of CO₂ exchange between the atmosphere and ecosystem and rely significantly on the parameterization scheme used in the model. In top-down methods, the bottom-up results are usually regarded as prior information about the CO₂ exchange processes and are optimized using the observations based on an inversion algorithm (mostly Bayesian methods) and an atmospheric transport model. The uncertainties in top-down methods can be attributed to three aspects: errors and the limited coverage of the observations, and errors in the atmospheric transport models. The existing in situ sites of atmospheric CO₂ can measure CO₂ mole fractions with high precision and a high temporal resolution; however, their sparse and uneven distribution limits their application in carbon cycle studies [4,5]. In recent years, space-based observations of CO₂ have provided unprecedented spatial coverage, which can significantly reduce the uncertainties in surface flux estimations [6,7]. The column-averaged dry-air mole fraction of CO₂ (XCO₂) retrieved from satellite spectra is relatively insensitive to vertical transport and mixing and also covers a larger geographical area [8,9]. The Greenhouse Gases Observing Satellite (GOSAT) launched in January 2009 is the first satellite dedicated to greenhouse-gas-monitoring [10]. The Orbiting Carbon Observatory 2 (OCO-2) is the second satellite dedicated to CO₂ monitoring, and was launched in July 2014 [11,12]. GOSAT measures radiance spectra with a Fourier transform spectrometer that has a wide spectral coverage ranging from shortwave infrared (SWIR) to thermal infrared (TIR), while OCO-2 uses an imaging grating spectrometer to record high-resolution spectra of reflected sunlight in the relevant bands. Compared to GOSAT, OCO-2 was designed to measure XCO₂ with enhanced spatial resolution and precision, which enables it to be a great data source in carbon cycle research [13].

Currently, satellite XCO₂ retrievals are being widely used to infer information about CO₂ sources and sinks, which can be implemented using atmospheric inverse models [14–21], where surface fluxes are optimally estimated by minimizing mismatches between satellite and ground-based observations and model simulations. However, the CO₂ flux inversion, particularly the regional flux inversion, requires satellite XCO₂ retrievals with high accuracy and precision because small biases in the retrieved XCO₂ distribution could be misinterpreted as evidence of CO₂ fluxes [2,14,18,21–25]. The threshold of the biases for XCO₂ is an important quantity in the carbon cycle research. Miller et al. [26] concluded that XCO₂ precision of 1–2 ppm is needed at regional scales to improve our knowledge of carbon cycle phenomena, but the geographic XCO₂ biases at regional to continental scales will have the largest impact on the inferred CO₂ surface fluxes. Buchwitz et al. [22] mentioned that the threshold requirement is 0.5 ppm for inverse modeling schemes. Therefore, the quality of different satellite XCO₂ retrievals must be continuously and carefully validated to ensure the quality of retrievals before application. To validate XCO₂ retrievals from space-borne instruments, the most effective method is comparing these retrievals with measurements from the Total Carbon Column Observing Network (TCCON), which is a network composed of ground-based Fourier transform spectrometers recording direct solar spectra in the near-infrared (NIR) bands. Since their measurements are minimally affected by land surface properties and aerosols, accurate and precise XCO₂ can be retrieved from the TCCON spectra [27,28]. Although in recent years there have been many studies validating satellite retrievals against TCCON observations [29–36], most publications focus on a single satellite, and the data used and the time period are limited. Because of their different satellite instrument and retrieval errors and the degradation of instruments with time, the latest and complete series of XCO₂ products still need to be carefully evaluated to ensure their consistent good quality before application in CO₂ flux inversion inversions. The enhanced observational coverage of a single satellite is still not sufficient for the CO₂ flux inversion problem because of the large gaps across satellite tracks and the long revisit time. With increasingly more carbon satellites being launched and in orbit, the joint use of different carbon satellite retrievals becomes an important challenge [37]. Actually, the XCO₂ retrievals from GOSAT and OCO-2 were calibrated separately before and after launch, and their calibration standards are in good agreement. However, the onboard calibration sources are limited and the calibration campaigns are always conducted over the same calibration targets in predetermined orbits, and the calibration

is always conducted around the summer solstice [37]. Therefore, the continuous cross-validation between GOSAT and OCO-2 XCO₂ retrievals is crucial to assess their consistency and potential for joint utilization.

In CO₂ flux inversions, in addition to the bias of XCO₂ retrievals, the errors caused by atmospheric transport models also account for the uncertainties in inferred surface fluxes [38]. In addition, the model grids are usually coarse and have different representative abilities with satellite observations [39]. Therefore, it is essential to analyse the spatio-temporal distribution and causes of the differences between modeled CO₂ mole fractions and satellite retrievals to assess the uncertainty in the model transports results and develop an appropriate observation operator used for CO₂ flux inversion [40]. Although several studies have compared GOSAT and model simulations [35,36,41,42], most researchers focus on a short period from many years ago and there is little research published comparing OCO-2 retrievals with model simulations. In this study, our objective is to explore the potential of XCO₂ retrievals from GOSAT and OCO-2 to be jointly used for CO₂ surface flux inversion analysis. We first evaluate the consistency of the XCO₂ retrievals from GOSAT, OCO-2 and TCCON. Then, we create a consistent combined dataset for inversion application in our future work. This dataset is also compared with long-term model data to assess its spatial and temporal components and assess its ability to characterize the carbon cycle.

The rest of the paper is organized as follows. Section 2 describes the datasets and methods used for comparison. The satellite data coverage, the inter-comparison among GOSAT, OCO-2 and TCCON and the comparison between XCO₂ calculated from the CarbonTracker transport model 5 (TM5) and that retrieved from GOSAT and OCO-2 are discussed in Section 3. Section 4 presents conclusions on the validation results and discussions on the joint usage of the GOSAT and OCO-2 data.

2. Materials and Methods

2.1. GOSAT

GOSAT, which was launched in January 2009, is the first satellite mission with a high spectral resolution and a wide spectral coverage dedicated to monitoring the concentrations of the main atmospheric greenhouse gases (i.e., CO₂ and methane (CH₄)). The GOSAT spacecraft is in a sun-synchronous, 98° inclination orbit at an altitude of 666 km, with a local descending node time between 12:45 p.m. and 13:15 p.m. and a revisit cycle of three days. The observation instruments on-board the satellite are the Thermal and Near-infrared Sensor for carbon Observation Fourier Transform Spectrometer (TANSO-FTS) and the TANSO-Cloud and Aerosol Imager (TANSO-CAI). The FTS observes solar radiation reflected by the Earth's surface and atmosphere in three SWIR bands which are near 0.76, 1.6, and 2.0 µm. The thermal radiation is observed at a wide TIR band spanning 5.5–14.3 µm which is not used here. The instantaneous field of view (IFOV) of the TANSO-FTS is 15.8 mrad, which corresponds to a circular footprint with an approximate 10.5 km diameter at nadir. TANSO-CAI images characterize cloud and aerosol properties in the field of view of the TANSO-FTS to filter out the cloud-contaminated footprints. Currently, several algorithms have been developed to retrieve XCO₂ from the TANSO-FTS/GOSAT observation spectra. Most approaches are based on optimal estimations given by Rodgers (Rodgers 2000). The GOSAT XCO₂ data used in this study are retrieved using the National Aeronautics and Space Administration (NASA) algorithm of Atmospheric CO₂ Observations from Space (ACOS), which is a full-physics XCO₂ retrieval algorithm described completely in O'Dell et al. [24]. This study used the retrieved GOSAT XCO₂ data from the ACOS v7.3 Lite data product (daily datasets with bias correction and warn levels). We used nadir land observations and ocean glint observations that are taken in high gain; medium gain over land has not been bias corrected due to lack of sufficient collocated validation data and hence these soundings are not included in the "Lite" files. The temporal coverage is from July 2009 to May 2016, and the data are held by the Goddard Earth Science Data Information and Services Centre (GES DIS, <https://disc.gsfc.nasa.gov/datasets?project=OCO>). We used a quality flag of 0 to filter the data.

2.2. OCO-2

OCO-2 is NASA's first satellite dedicated to monitoring CO₂, which was launched on 2 July 2014. The OCO-2 satellite was launched into the 705 km Afternoon Constellation (A-Train). This near-polar (98.2° inclination), sun-synchronous orbit has a 98.8 min period, a 16 day/233 orbit ground track repeat cycle and an equator crossing time near 1:36 p.m. The OCO-2 instrument incorporates three co-boresighted, long-slit, imaging grating spectrometers optimized for observing the molecular oxygen (O₂) A-band at 0.765 µm and the CO₂ bands at 1.61 and 2.06 µm. The footprint dimensions are determined by a cross-track IFOV of 0.1° and integration time of 0.333 s. For nadir observations, this yields four to eight cross-track footprints along the spectrometer slit with dimensions of 1.29 km by 2.25 km. The retrieval algorithm used to create the Build 7 ACOS data product is consistent with that used to create the OCO-2 v7r data product used in this study, which allows for the comparison of ACOS and OCO-2 data without having to consider algorithm differences. In this study, the retrieved XCO₂ from the OCO-2 v7r Lite product was also obtained from GES DIS (<https://disc.gsfc.nasa.gov/datasets?project=OCO>), and the data coverage is from September 2014 to July 2017. Similar to GOSAT/ACOS, we used a quality flag of 0 to filter the data.

2.3. TCCON

TCCON is a global network of ground-based Fourier transform spectrometers that record NIR solar absorption spectra. Since their measurements are minimally affected by aerosols and various surface properties, the column-averaged abundances of CO₂, CH₄, N₂O, HF, CO, H₂O, and HDO retrieved from these spectra are relatively accurate and precise [27–29]. TCCON started in 2004, and it has 23 instruments currently in operation around the globe, with seven former sites. The scientific goal of the TCCON is to improve our understanding of the carbon cycle, and since retrievals from the TCCON are more precise and accurate than space-based instruments, it is currently an ideal validation dataset for the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY), GOSAT and OCO-2. The latest version (GGG2014) of the TCCON dataset was used in this study. We applied a four-fold standard difference method to further filter the data; that is, individual data points for which the differences with the neighbouring observations were outside the range of $m \pm 4\sigma$ were selected as outliers, where m represents the mean value and σ represents the standard deviation in the differences of the XCO₂ retrievals. Figure 1 shows the location of the operational, former and potential TCCON sites around the globe.

Figure 1. Locations of the operational, previous and potential TCCON sites.

2.4. CarbonTracker

CarbonTracker (CT) is a CO₂ data assimilation system developed by the National Oceanic and Atmospheric Administration (NOAA, Silver Spring, MD, USA) that uses the observations of the atmospheric CO₂ mole fraction and the TM5 model to simulate and estimate the surface fluxes of CO₂ ([43], with updates documented at <http://carbontracker.noaa.gov>). In this study, we used the modeled 3D CO₂ mole fractions by the CT2017 to quantify the data consistency between the satellites and the model.

CT2017 provides global 3D CO₂ mole fractions with 25 vertical levels, a 3° × 2° longitude-latitude grid, and a 3-h temporal resolution. To compare with the retrieved XCO₂ from GOSAT and OCO-2, the model-simulated CO₂ profiles were converted into XCO₂ using the averaging kernel and a priori profiles of the satellites according to Connor et al. [44]:

$$XCO_2^m = XCO_2^a + \sum_j^n h_j a_j (H(x) - y_a)_j, \quad (1)$$

where $H(x)$ represents the observation operator that maps the model-simulated CO₂ profiles to the GOSAT or OCO-2 XCO₂ observation space, XCO_2^m represents the modeled XCO₂, XCO_2^a represents the a priori XCO₂, a represents the column averaging kernel of the satellite, and h represents the pressure weighting function, y_a is the model simulated CO₂ profiles and j indicates the j th level of total n levels.

2.5. Spatiotemporal Collocation Criterion

In order to select a set of near-simultaneous XCO₂ data from satellite and TCCON measurements for comparison, we used the geophysical collocation criteria of temporal-spatial separation within ±110 km and ±30 min. For each TCCON observation, the satellite scans are selected using the collocation criteria, then the duplicated and high-frequent collocations were averaged every 1 h as most of the TCCON XCO₂ data are reported every few minutes. Before the matching process, we discarded the ocean glint measurements of GOSAT and OCO-2 data for matching with TCCON land observations, since the TCCON sites are located on land.

For cross-comparison between GOSAT and OCO-2 XCO₂, we selected the OCO-2 XCO₂ within each GOSAT footprint which is a 10.5 km diameter circle since the much larger GOSAT footprint can cover dozens of OCO-2 footprints in nadir or glint mode, and hundreds of OCO-2 footprints in target mode [37]. Then, the selected OCO-2 data were averaged. In this way, the collected collocations between GOSAT and OCO-2 can be considered as observations at the same location and thus minimizing the comparison uncertainties brought by the spatial separation. The temporal coincidence criterion used here was ±1 h.

TCCON and GOSAT/OCO-2 XCO₂ have different a priori profiles and averaging kernels, which describe the sensitivity of a retrieval algorithm to the true state throughout the atmosphere [45,46]. Recent research has demonstrated that the effect of column averaging kernels on GOSAT and OCO-2 XCO₂ is relatively negligible when compared with its measurement accuracy, and direct comparison is applicable in the validation of satellite's measurements site [13,34]. Therefore, similar to several works, this comparison has not taken into account the effect of the different averaging kernels and a priori between the remote sounders [13,34,41,47].

3. Results

3.1. Spatial Coverage of GOSAT and OCO-2 Observations

Despite the accuracy of the XCO₂ retrievals, the uniformity of the data distribution is also very important in data assimilation. However, due to cloud contamination and other poor conditions, a number of observations are identified as bad data, leaving the remaining data unevenly distributed.

The combination of data from multiple satellites can enhance data coverage, especially in polluted and tropical areas.

Figures 2 and 3 show the spatial coverages of the GOSAT and OCO-2 retrievals within the first three days in July and December 2015, respectively. In every 2×2.5 grid cell, if it contains a useful satellite retrieval, then it is filled with a color (GOSAT is blue, while OCO-2 is green). The grid coverage rate is increased by combining the two satellites (Table 1). During the first three days in July 2015, the grid coverage fraction is 5.2% for GOSAT, 9.8% for OCO-2, and 13.9% for the joint dataset. During the first three days in December 2015, the grid coverage fraction is 4.3% for GOSAT, 9.1% for OCO-2, and 12.6% for the joint dataset. Although the joint dataset has utilization potentiality in carbon cycle research, such as carbon flux inversion, the XCO_2 accuracy are still the most important factor influencing the inversion results that needs to be continually validated and improved.

Figure 2. Map of the data coverages of GOSAT and OCO-2 within the first three days in July 2015.

Figure 3. Map of the data coverages of GOSAT and OCO-2 within the first three days in December 2015.

Table 1. Fractions of local grid coverage by GOSAT, OCO-2 and the joint dataset at a resolution of 2° latitude $\times$ 2.5° longitude.

Time	GOSAT Coverage	OCO-2 Coverage	Joint Dataset Coverage
1–3 July 2015	5.2%	9.8%	13.9%
1–3 December 2015	4.3%	9.1%	12.6%

3.2. The Inter-Comparison of GOSAT, OCO-2 and TCCON

3.2.1. Validation of the OCO-2 and GOSAT XCO_2 Products Using TCCON Data

The time range of the GOSAT/ACOS XCO_2 product is from July 2009 to May 2016, and the time range of the OCO-2 products is from September 2014 to July 2017. The latest version of the TCCON data product used here (GGG2014) covers a time range from June 2004 to the end of 2017. Table 2 shows the time coverage of each TCCON site and the number of collocations with the GOSAT/ACOS and OCO-2 retrievals using the ± 110 km and ± 30 min spatio-temporal collocation criteria described in Section 2.5.

As a result, there are a total of 2488 matched observations between GOSAT and TCCON, and the number of collocations in the mid-latitudes of the Northern Hemisphere is the largest, which can be seen from the colours of the scattered collocations in Figure 4a. The mean bias $\pm$ standard deviation of differences is 0.24 ± 1.68 ppm, and the correlation coefficient is 0.95. For OCO-2, there are 1009 matched observations with the TCCON, and the number of collocations in the mid-latitudes of the Northern Hemisphere is also the largest. The mean bias $\pm$ standard deviation of differences is 0.34 ± 1.57 ppm, and the correlation coefficient is 0.92 (Figure 4b). In high latitudes, particularly north of 60° N, the retrievals of OCO-2 are visibly larger than those of the TCCON (red points in Figure 4b). As shown in Figure 4, an orthogonal linear regression (OLR) was performed instead of an ordinary least squares (OLS) regression, with the TCCON XCO_2 as the independent variable and OCO-2 XCO_2 as the dependent variable. These settings are chosen because an OLR is warranted if the measurement errors in both variables are comparable, and thus both variables are treated symmetrically. However, an OLS regression assumes no measurement errors in the independent variable and generally yields a relatively smaller slope value than the OLR [48]. In Figure 4a,b, the fitting line of the OLR is very close to the one-to-one line, indicating that the mean differences between the satellite retrievals and TCCON XCO_2 are very small. In general, although the satellites slightly overestimated the XCO_2 mole fractions compared to the TCCON, the satellite XCO_2 measurements are generally in good agreement with the TCCON data, indicating that the satellite products with good quality flags are well calibrated with the TCCON data.

Table 2. Information on the TCCON sites used in the comparison with the GOSAT/ACOS and OCO-2 retrievals. The number of collocations with both satellites using the method described in Section 2.5 is also listed.

Name	Temporal Coverage	Location (Lat, Long)	Reference	Number of Collocations with GOSAT	Number of Collocations with OCO-2
Sodankyla	05/2009–10/2017	67.37, 26.63	Kivi et al. [49]	13	20
East trout lake	10/2016–10/2017	54.36, −104.99	Wunch et al. [50]	0	20
Bialystok	03/2009–02/2017	53.23, 23.02	Deutscher et al. [51]	29	36
Bremen	01/2007–02/2017	53.10, 8.85	Notholt et al. [52]	14	9
Karlsruhe	04/2010–04/2016	49.10, 8.44	Hase et al. [53]	34	38
Paris	09/2014–11/2016	48.85, 2.36	Te et al. [54]	15	21
Orléans	08/2009–02/2017	47.97, 2.11	Warneke et al. [55]	60	35
Garmisch	07/2007–12/2017	47.48, 11.06	Sussmann et al. [56]	50	13
Parkfalls	06/2004–10/2017	45.94, −90.27	Wennberg et al. [57]	88	55
Rikubetsu	11/2013–02/2017	43.46, 143.77	Morino et al. [58]	11	5
Indianapolis	08/2012–12/2012	39.86, −86.00	Iraci et al. [59]	5	0
Fourcorners	03/2013–10/2013	36.80, −108.48	Dubey et al. [60]	7	0
Lamont	07/2008–10/2017	36.60, −97.49	Wennberg et al. [61]	304	179
Anmeyondo	02/2015–11/2016	36.54, 126.33	Goo et al. [62]	8	11
Tsukuba	08/2011–02/2017	36.05, 140.12	Morino et al. [63]	183	62
Edwards	07/2013–08/2016	34.96, −117.88	Iraci et al. [64]	347	101
Jpl	05/2011–02/2018	34.20, −118.18	Wennberg et al. [65]	172	7
Pasadena	09/2012–10/2017	34.14, −18.13	Wennberg et al. [66]	508	138
Saga	07/2011–09/2017	33.24, 130.29	Kawakami et al. [67]	65	26
Izana	05/2007–07/2016	28.30, −16.48	Blumenstock et al. [68]	0	3
Manaus	10/2014–06/2015	−3.21, −60.60	Dubey et al. [69]	0	2
Ascension	05/2012–12/2017	−7.92, −14.33	Feist et al. [70]	0	8
Darwin	08/2005–11/2016	−12.43, 130.89	Griffith et al. [71]	175	69
Réunion Island	16/2011–11/2017	−20.90, 55.49	De Mazière et al. [72]	0	24
Wollongong	06/2008–02/2017	−34.41, 150.88	Griffith et al. [73]	204	77
Lauder01	02/2010–08/2017	−45.04, 169.68	Sherlock et al. [74]	166	114
Lauder02	06/2004–12/2010	−45.05, 169.68	Sherlock et al. [75]	30	0

Figure 4. Scatter plot of the collocations of (a) TCCON and GOSAT XCO₂ and (b) TCCON and OCO-2 XCO₂ using the ± 110 km and ± 30 min coincidence criteria. The colors in both panels represent the latitudes of the TCCON sites. The dotted line represents the one-to-one line, and the red solid line represents the OLR, with the corresponding regression formula shown in the figure. In all figures, N represents the number of matched collocations, β represents the mean bias of the matched data pairs, σ represents the standard deviation, and ρ represents the correlation coefficient of the matched data pairs.

Since the TCCON sites are located dispersedly in various geographical environments, the data volume may have large differences. Additionally, the XCO₂ mole fractions in the Northern and Southern Hemispheres have different characteristics and seasonal patterns; therefore, we categorize the sites into different latitudinal zones to validate the measurements. Here, we divide the TCCON sites into four latitudinal zones based on previous works but with few differences (see Figures 5 and 6) noting that the 0–28°N zone does not have a TCCON site.

Figures 5 and 6 show the scatter plots of the collocations of the TCCON with GOSAT and TCCON with OCO-2, respectively. Their collocations are in the four latitude zones that are binned around the TCCON sites. Each color in the figures represents one TCCON site. The OCO-2 mole fractions match more XCO₂ observations that are higher than 400 ppm while GOSAT capture more XCO₂ observations below 400 ppm. The mean bias between the satellite and TCCON XCO₂ data are positive in most zones, indicating that the XCO₂ via satellites is slightly overestimated compared to that via the TCCON. The standard deviation of differences between the OCO-2 and TCCON XCO₂ vary from 1.09 to 1.59 ppm, while, for GOSAT, the standard deviation values vary from 1.53 to 1.72 ppm, indicating that the OCO-2 retrievals are closer to the TCCON data than the GOSAT retrievals. For GOSAT, the differences in collocations between the GOSAT and TCCON XCO₂ are the largest over 28° N–40° N, with a mean bias $\pm$ standard deviation of differences of 0.39 ± 1.72 ppm. Figure 7 shows a scatter plot of the collocations between the TCCON and GOSAT XCO₂ over 28° N–40° N, where the different colors represent the dates of the measurements. Similar to Figure 5b, the difference between the GOSAT and TCCON XCO₂ in the mid-latitudes of the Northern Hemisphere is the greatest among all latitudes. Additionally, the differences increase with time and become larger in recent years compared to the first two years after the launch of GOSAT, and the increased differences have no relationship with the TCCON sites. As is shown below, no discernable time dependence of the differences between TCCON and OCO-2 XCO₂. Figure 8 also shows the same result, which may result from instrument degradation on board GOSAT.

Figure 5. Scatter plots of the collocations of the TCCON and GOSAT XCO₂ in four latitude zones: (a) 40° N–85° N; (b) 28° N–40° N; (c) 0–40° S; and (d) 40° S–60° S. The vertical error bars represent the standard deviations of the GOSAT data, while the horizontal bars represent the standard deviations of the TCCON data. Each TCCON site is represented by a certain color. The latitudes are binned around the TCCON sites.

Figure 6. Scatter plots of the collocations of the TCCON and OCO-2 XCO₂ in the four latitude zones that are binned around the TCCON sites: (a) 40° N–85° N; (b) 28° N–40° N; (c) 0–40° S; and (d) 40° S–60° S. The vertical error bars represent the standard deviations of the OCO-2 data, while the horizontal bars represent the standard deviations of the TCCON data. Each TCCON site is represented by a certain color.

Figure 7. Scatter plot of the collocations of the TCCON and GOSAT XCO₂ over 28° N–40° N, which is similar to the second panels in Figure 5b but with the colors representing the change in time instead of the TCCON sites. The temporal range is from September 2009 to May 2016.

Figure 8 shows a comparison of the time series and the differences in the GOSAT/OCO-2 and TCCON collocations in the Northern and Southern Hemispheres. In the Northern Hemisphere, the two satellites and the TCCON XCO₂ measurements have consistent seasonal fluctuations and an overall increasing trend. The XCO₂ mole fractions is the lowest in September and the highest in spring (March–May) throughout the year. This seasonal pattern suggests much higher anthropogenic emissions in winter and a more natural uptake of CO₂ in summer with a lag effect. The differences between the satellite and TCCON XCO₂ show a seasonal dependence that is relatively larger in summer and smaller in autumn, indicating that the satellite measurements in summer have relatively larger uncertainties. In addition to the seasonal dependence, the differences between GOSAT and TCCON XCO₂ become larger with time and even more obvious in the years of 2014–2015. The increased differences are particularly significant in the mid-latitudes of the Northern Hemisphere and can reach 3–5 ppm, which is much larger than it was during the first two years after the satellite was launched. It is not obvious in other latitudes and the differences between OCO-2 and TCCON XCO₂ data also have no time dependence. Liang et al. [13] found that the total difference between the GOSAT and TCCON XCO₂ is greater after 2014 than it was before 2014. In that study, the GOSAT retrieved data are performed via another retrieval algorithm (i.e., the National Institute for Environmental Studies (NIES) algorithm [76]), indicating that the increasing differences are independent of the retrieval method. Therefore, future GOSAT retrievals should be continuously validated to ensure data quality. In the Southern Hemisphere, seasonal fluctuations are not significant, with only an increasing trend evident. The differences between the satellite and TCCON XCO₂ do not clearly show any time dependency, which may partly be due to the relative homogeneous environment.

Figure 8. Time series of the satellite XCO_2 , the coinciding TCCON data and their differences. The right panel shows the time series of the coincidences between the GOSAT XCO_2 and TCCON soundings in (a) the Northern Hemisphere and (b) Southern Hemisphere and (c) the difference between the GOSAT and TCCON XCO_2 ($\Delta XCO_2 = \text{GOSAT} - \text{TCCON}$). The left panel shows the time series of the coincidences of the OCO-2 XCO_2 and TCCON soundings in the (d) Northern Hemisphere and (e) Southern Hemisphere and (f) ΔXCO_2 (OCO-2 – TCCON).

3.2.2. The Cross Comparison between the GOSAT and OCO-2 XCO_2

For cross-comparison, we used XCO_2 between September 2014 and May 2016 since the GOSAT/ACOS V7.3 Lite data are currently available before May 2016. In this section, 10.5 km circle and ± 1 h separation limits were used as the coincidence criteria, which was described in Section 2.5.

Figure 9 shows the scatter plot of the collocations between the GOSAT and OCO-2 XCO_2 . There are 566 matching points. The mean bias $\pm$ standard deviation of differences is 0.21 ± 1.3 ppm, and the correlation coefficient is 0.89. An OLR was performed with GOSAT XCO_2 as the independent variable and OCO-2 XCO_2 as the dependent variable. The colors represent the densities of the collocations, and the denser collocations are centered on the one-to-one line.

Figure 10 shows a global map of the differences between the GOSAT and OCO-2 XCO_2 at the collocated points. In most regions, the differences are small and within 2 ppm, with GOSAT XCO_2 being slightly underestimated with respect to OCO-2 XCO_2 . While there are larger differences over Asia than other regions, they remain within ± 5 ppm. Figure 11 shows the time series of ΔXCO_2 (i.e., $XCO_2_{\text{GOSAT}} - XCO_2_{\text{OCO-2}}$) between GOSAT and OCO-2. The time series of ΔXCO_2 indicates that there is no significant time-dependent variation in ΔXCO_2 , and the discrepancies between OCO-2 and GOSAT are small (within ± 2 ppm), indicating that the systematic error between collocations is not obvious. The results are similar to those of [37], but this work applies a quality filter, and the biases are much smaller. The biases between OCO-2 and GOSAT may be primarily caused by the matching errors and retrieving errors. Based on the above analysis and to make full use of the data products from the two satellites, we can combine the GOSAT and OCO-2 good quality data and form a combined dataset for further research.

Figure 9. Scatter plot of the collocations between the GOSAT and OCO-2 XCO₂. Scatter density: the number of collocations in each bin of 20 × 20 bins.

Figure 10. The spatial variation in the differences between GOSAT and OCO-2.

Figure 11. The time series of ΔXCO_2 between GOSAT and OCO-2. The error bars indicate the standard deviation of ΔXCO_2 within each GOSAT IFOV. The green dotted lines represent the threshold value of ± 2 ppm.

3.3. Comparison of XCO₂ Satellite Retrievals with XCO₂ Computed from a Model

In this section, a comparison between the XCO₂ calculated from the CT2017 output and retrievals of GOSAT and OCO-2 is detailed.

First, we used the method and Equation (1) described in Section 2.4 to calculate the XCO₂ from the CT2017 for comparison with the XCO₂ retrievals from GOSAT and OCO-2. To conduct a spatial comparison, the daily along-track datasets were averaged over 2° × 2° (GOSAT) and 1° × 1° (OCO-2) latitude-longitude grids to calculate the monthly, seasonal and annual mean gridded datasets.

Figure 12 shows the global distribution of XCO_2 from GOSAT/ACOS and CT2017 and their differences in the four seasons during March 2015–February 2016. In summer and autumn, the GOSAT and CT2017 XCO_2 values and their spatial distributions are very similar. However, in spring and winter, there are larger, more visible differences, particularly in the extratropical latitudes of the Northern Hemisphere, with CT2017 XCO_2 values that are larger but have less significant spatial variations than those of the GOSAT XCO_2 , this even over small areas. In most regions, the CT2017 XCO_2 is slightly higher than GOSAT XCO_2 , while in northern Asia, the CT2017 XCO_2 is smaller than the GOSAT XCO_2 . In general, the characteristics of the GOSAT and CT2017 XCO_2 spatial distributions are similar, and the global map of ΔXCO_2 shows that the differences in most regions are within ± 2.5 ppm.

The XCO_2 scans of GOSAT in 2015 and the corresponding CT2017-modeled XCO_2 values at these observation points are compared in Figure 13. The total number of XCO_2 scans is 136,222 over the ocean, which is much larger than the 52,221 scans over land. Figure 13 clearly shows that the CT and GOSAT XCO_2 values are much closer over the ocean than those over land since there are some very large differences (greater than 5 ppm) over land. The mean biases $\pm$ standard deviations are (a) 0.43 ± 2.02 ppm over land and (b) 0.59 ± 1.14 ppm over the ocean. This result can be explained by the more dynamic sources and sinks over land, with the CO_2 mole fractions varying greatly with space and time. As a result, the uncertainties in the seasonal mean mole fractions are larger over land than the ocean, especially from the model results.

Figure 12. Global distributions of the GOSAT XCO_2 (left panel), CT2017-modeled XCO_2 (middle panel) and the differences between the CT2017 XCO_2 and GOSAT XCO_2 (right panel; $\Delta XCO_2 = XCO_2_{CT} - XCO_2_{GOSAT}$). Each row of panels, from top to bottom, subsequently represents spring, summer, autumn and winter.

The distribution characteristics of the XCO_2 values retrieved from OCO-2 are similar to those of the simulated XCO_2 using CT2017 over most regions. Over the desert zone of North Africa, the region of the Tibetan Plateau, and several other areas with high plateaus and mountain ranges, XCO_2 values simulated by CT2017 are significantly larger than those retrieved by OCO-2, particularly in spring and winter. In the Central African Rainforest, XCO_2 is slightly underestimated using CT2017 compared

to that retrieved by OCO-2 and GOSAT. Similar to Central Africa, XCO_2 in the Amazon Rainforest is slightly underestimated by CT2017 compared with that in the limited OCO-2 observations. These areas are important because they are large carbon sinks that can have significant impacts on the global carbon budget. In general, the differences in most regions are within ± 5 ppm, while, in some regions, such as deserts, plateaus and mountains, the differences can reach 5 ppm, and some are even much larger than that. Cogan et al. [47] also found the largest differences are observed over desert regions such as the Sahara and central Asia when comparing GEOS-Chem model result with GOSAT XCO_2 in the year 2010–2011. The differences over the ocean are smaller than those over land, as shown in Figure 14.

Figure 13. The scatter plots of the GOSAT and CT2017 XCO_2 (a) over land and (b) over the ocean. N represents the total number of GOSAT retrievals after data quality control in 2015.

Figure 14. Global distribution of the OCO-2 XCO_2 (left panel), CT2017-modeled XCO_2 (middle panel) and the differences between the CT2017 XCO_2 and OCO-2 XCO_2 (right panel; $\Delta XCO_2 = XCO_2_{CT} - XCO_2_{OCO-2}$). Each row of panels, from top to bottom, subsequently represents spring, summer, autumn and winter.

Figure 15 shows the scatter plots of the OCO-2 and CT XCO₂ over land and the ocean. The total number of XCO₂ scans was 6,645,124 over land, and 13,936,046 scans over the ocean. The mean biases $\pm$ standard deviations are (a) 0.48 ± 1.99 ppm over land and (b) 0.2 ± 0.98 ppm over ocean. The correlation between the OCO-2 and CT XCO₂ seems to be more scattered than that between the GOSAT and CT XCO₂, which is probably because OCO-2 provides more observations with a finer spatial resolution, while the CT model grids are coarse and lead to large uncertainties when interpolated to the OCO-2 observation space.

Figure 15. Scatter plots of the OCO-2 and CT XCO₂ (a) over land and (b) over the ocean. N represents the total number of OCO-2 retrievals after data quality control in 2015.

Apart from the comparison of the satellite and CT gridded XCO₂ data in 2015 on a global map, we also generated a time series from 2009 to 2016 to further access the consistency among the XCO₂ datasets. In addition, climate variability was calculated and analysed to evaluate the abilities of the datasets to characterize climate change. To make full use of the two satellite datasets, we combined the XCO₂ scans from both satellites together to form one data set. Then, the monthly and seasonal means of the globally gridded data were generated from the dataset for the XCO₂ climate trend analysis. Figure 16 shows the time series plots of the monthly mean XCO₂ in the Northern and Southern Hemispheres calculated from the satellites and the CT2017 globally gridded XCO₂ datasets. In the Northern Hemisphere, the values of the monthly mean XCO₂ are very close (the differences are almost zero) for all datasets, and the values have the same seasonal fluctuations and variation trends. During the period from September 2014 to the end of 2016, when OCO-2 and GOSAT are simultaneously in orbit, the merged dataset is more similar to the OCO-2 data than the GOSAT data because of the much larger number of observations by OCO-2 compared to GOSAT. The time series in the Northern Hemisphere shows a significant increasing trend and obvious seasonal fluctuations, which peak in April and May and reach a minimum in September. This result has lagged correlations with the CO₂ uptake of the enhanced terrestrial ecosystem and the concentrated anthropogenic CO₂ emissions in winter. However, for the Southern Hemisphere, there are no obvious seasonal fluctuations, and the values are always close to the lowest value in the Northern Hemisphere since they are less affected by human activity, particularly in extratropical latitudes. The monthly mean XCO₂ from the satellites is slightly different than that from CT2017, with peaks slightly higher and minimums smaller than those of the monthly mean time series calculated from the CT2017 XCO₂ datasets.

Figure 16. Monthly mean XCO_2 from satellites and CT2017 in (a) the Northern Hemisphere and (b) Southern Hemisphere. The word “Merge” in the legend indicates the combination of the GOSAT and OCO-2 scans.

Figure 17 shows the growth rates of the global seasonal mean XCO_2 from the merged satellite dataset and the CT2017 model dataset. The growth rates computed from the satellite dataset increased significantly in autumn of 2015, continued to increase and maintained high values from autumn 2015 to spring 2016, and then began to slow down after autumn 2016. The supplementary OCO-2 data in 2017 show that the growth rates return to normal in 2017 (not shown here). The large El Niño during 2015 and 2016 was responsible for the record sustained global growth rates in atmospheric CO_2 , which resulted in the enhanced rise of XCO_2 in 2015 and 2016. The growth rates computed from the CT2017 XCO_2 dataset showed a delayed increase that occurred in spring of 2016. However, the growth rates were close in 2016, which reached 3 ppm per year.

Figure 17. Plots of the global seasonal mean XCO_2 growth rates inferred from (a) the merged satellite data and (b) the CT2017 data.

We used the seasonal Kendall (S-K) method to compute the mean trend in XCO_2 from the seasonal mean XCO_2 from June 2009 to the end of 2016 in each $1^\circ \times 1^\circ$ grid. The S-K method [77] is derived from the Mann–Kendall method (M–K) and is superior to the M–K method because the S-K method considers the seasonal fluctuation of datasets. In this study, we used the S-K test to account for the seasonality in atmospheric CO_2 by computing the M–K test on each of the seasons separately and then combining the results. Figure 18 shows the global maps of Sen's slope calculated from the seasonal mean dataset of satellite-retrieved XCO_2 and the seasonal dataset of CT2017-modeled XCO_2 using the S-K method. The trend calculated from the satellite dataset was slightly more obvious than that from the CT2017 dataset in some mid-latitude regions, such as East America, North China and western Europe, while, in the Southern Hemisphere, the trend values calculated from the satellite dataset were smaller than those from the CT2017 dataset. Nevertheless, the trends from both datasets were generally very similar, with values ranging from 2–2.6 ppm per year. In addition, despite the long-range transport of CO_2 by atmospheric circulation, the trend slopes in the Northern Hemisphere were still apparently larger than those in the Southern Hemisphere.

Figure 18. Global map of the mean trend in XCO_2 calculated from (a) the satellite seasonal mean XCO_2 dataset and (b) the CT-modeled XCO_2 seasonal dataset using the S-K method. Sen's slope represents the trend slope calculated using the S-K method.

4. Conclusions and Discussion

The estimation of carbon sources and sinks requires precise XCO_2 observations, and these data need to be validated before their application because of satellite instrument errors, retrieval errors and the instrument degradation. Since more carbon cycle satellites have been launched or will be launched, the continuous cross-validation of GOSAT and OCO-2 XCO_2 measurements is crucial to assess their consistency and potential for joint utilization. The assessment of the spatio-temporal components of satellite XCO_2 retrievals and model outputs can help us to develop appropriate observation operators in carbon cycle data assimilation.

First, we validated the GOSAT/ACOS and OCO-2 XCO_2 retrieval products using the ground-based TCCON. The satellite XCO_2 measurements are generally in good agreement with the TCCON data, with a mean bias $\pm$ standard deviation of differences of 0.24 ± 1.68 ppm for GOSAT and 0.34 ± 1.57 ppm for OCO-2. The results showed that the differences between the GOSAT and

TCCON XCO₂ increased with time and became larger in recent years than the first two years after the launch of GOSAT. The increasing differences are particularly significant in the mid-latitudes of the Northern Hemisphere, which can reach 3–5 ppm. Liang et al. [13] also found that the total difference between the GOSAT and TCCON XCO₂ is greater after 2014 than it was before 2014. Their work showed that the mean bias $\pm$ standard deviation of differences are -0.4107 ± 2.216 ppm for GOSAT (slightly larger than this study which may be mainly due to that they use a different source of data and a different collocation criteria with us) and 0.2671 ± 1.56 ppm for OCO-2. Therefore, future retrievals must be continuously validated to ensure data quality. Then, we evaluated the consistency of the two satellite observations through cross comparisons. The retrievals from the two satellites agree well, with a small mean bias $\pm$ standard deviation of differences of 0.21 ± 1.3 ppm. The results are similar to those of [37], but this work applies a quality filter, and the biases are much smaller. The differences between the two satellite retrievals are independent of time, indicating that the systematic error between the collocations is not obvious, and the biases between OCO-2 and GOSAT may be primarily caused by matching errors and retrieval errors. Therefore, we think it is possible to combine the GOSAT and OCO-2 good quality data for CO₂ surface flux inversion studies.

Finally, the differences between the CT2017-modeled XCO₂ data and the satellite retrievals were analyzed. The CT2017 XCO₂ spatial variation is much less significant than the variation in the retrievals from the two satellites because of the denser observations and higher resolutions of the satellites, which can reflect the actual impact of the surface carbon fluxes (particularly for the retrievals from OCO-2). The differences between GOSAT and CT2017 XCO₂ are within ± 2.5 ppm in most areas. Overall, the differences between GOSAT and CT2017 XCO₂ are larger over land than over the ocean, with mean biases $\pm$ standard deviations of 0.43 ± 2.02 ppm and 0.59 ± 1.14 ppm and correlation coefficients of 0.71 and 0.73, respectively. The differences between the OCO-2 and CT2017 XCO₂ over land are larger than those between GOSAT and CT, while the OCO-2 retrievals and CT2017 XCO₂ are much closer over the ocean. The differences between the OCO-2 and CT2017 XCO₂ are within ± 5 ppm in most areas. The OCO-2 and CT2017 XCO₂ differ more greatly, which is probably because OCO-2 has a much finer spatial resolution, while the model grid is much coarser; therefore, interpolating the modeled 3D CO₂ mole fractions to the OCO-2 observation space can cause large errors and uncertainties. Therefore, the representative errors of the model and the satellite observations have great impact and must be described appropriately during carbon satellite data assimilation. In addition, we combined the GOSAT and OCO-2 XCO₂ data and conducted an analysis on carbon cycle climate changes and variations based on the combined dataset. The trend in the time series of the combined dataset is almost the same as that in the result from the CT2017-modeled XCO₂ dataset, and both datasets well characterize the significant increase in atmospheric CO₂ under the impact of the large El Niño during 2015 and 2016.

In Section 3.3, we created a joint dataset of the XCO₂ retrievals from GOSAT and OCO-2 and preliminarily analyzed its applicability in carbon cycle research. The joint dataset is also made for the carbon cycle data assimilation system to improve the estimation accuracy of CO₂ surface fluxes in our following work. The joint dataset is currently made by combining the along-track satellite retrievals with the recommended quality flag. These retrievals are ranked in chronological order, with each retrieval including information about the satellite (e.g., sounding ID). To be utilized in data assimilation, the data quality is further controlled by filtering under a threshold, such as the mean value $\pm$ three or four standard deviations in each track. For the coinciding retrievals, since OCO-2 has a higher observation resolution and a finer spatial resolution than GOSAT, we can choose to only retain the OCO-2 retrievals or retain all collocations since the assimilation algorithm will assign different weights to these data according to their uncertainties.

The main purpose of these carbon satellites is to obtain information on surface sources and sinks; therefore, the improvements in the retrieval algorithm and the quality control of the retrievals, as well as the combination of observations retrieved from different instruments on the basis of the existing space-based datasets, are very important to improve the accuracy of the estimated CO₂ surface fluxes.

In this study, the comparison of the retrievals (with good quality flags) from different instruments shows good consistency and a possibility for them to be jointly used. The comparative analysis with the model data is helpful in designing the observation operator used in carbon cycle data assimilations and flux inversions.

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