

Comparisons of OCO-2 satellite derived XCO₂ with *in situ* and modeled data over global ocean

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Abstract

Atmospheric CO₂ is one of key parameters to estimate air-sea CO₂ flux. The Orbiting Carbon Observatory-2 (OCO-2) satellite has observed the column-averaged dry-air mole fractions of global atmospheric carbon dioxide (XCO₂) since 2014. In this study, the OCO-2 XCO₂ products were compared between *in-situ* data from the Total Carbon Column Network (TCCON) and Global Monitoring Division (GMD), and modeling data from CarbonTracker2019 over global ocean and land. Results showed that the OCO-2 XCO₂ data are consistent with the TCCON and GMD *in situ* XCO₂ data, with mean absolute biases of 0.25×10^{-6} and 0.67×10^{-6} , respectively. Moreover, the OCO-2 XCO₂ data are also consistent with the CarbonTracker2019 modeling XCO₂ data, with mean absolute biases of 0.78×10^{-6} over ocean and 1.02×10^{-6} over land. The results indicated the high accuracy of the OCO-2 XCO₂ product over global ocean which could be applied to estimate the air-sea CO₂ flux.

Key words: XCO₂, OCO-2, comparison, *in situ*, modeling data

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1 Introduction

Due to the utilization of fossil fuels and changes in land use, atmospheric CO₂ has continued to increase since the industrial revolution, which has profound impact on earth carbon cycle and global warming (IPCC, 2013). Accurate observations of atmospheric CO₂ with high spatiotemporal resolution are the basis for estimating air-sea CO₂ flux (Bai et al., 2015; Song et al., 2016), understanding long-term changes and improving our ability to predict and mitigate climate change (Intergovernmental Panel on Climate Change, 2007; Jenkinson et al., 1991). Understanding the global atmospheric carbon dioxide concentration, especially the atmospheric carbon dioxide change over the ocean, is an important reference for many global climate changes above. Currently, there are several ways to obtain dry-air mole fractions of atmospheric CO₂ (XCO₂), including *in situ* measurements, remote sensing and modeling simulation. *In situ* measurements generally provide the best quality CO₂ concentrations, but the number of ground-based sites is limited, resulting in the absence of data in many global areas, especially in oceanic regions (Bousquet et al., 2006; Eldering et al., 2017). In contrast, spaceborne detection is the most effective technical method to observe atmospheric XCO₂ with long time series and global cover-

age. For example, the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography launched in 2002 was the first space-based instrument to retrieve atmospheric XCO₂ (Bovensmann et al., 1999; Buchwitz et al., 2007). Launched in April 2009, the Greenhouse Gases Observing Satellite (GOSAT) provides a more accurate atmospheric XCO₂ product, at a precision of around 0.6% (Cogan et al., 2012; Joiner et al., 2011; Yokota et al., 2009), as does GOSAT-2, which was launched in October 2018. Especially, NASA launched the Orbiting Carbon Observatory-2 (OCO-2) on 2 July 2014 to provide an atmospheric XCO₂ product with higher accuracy (Crisp, 2015). In addition, China launched TANSAT satellite in December 2016 to measure atmospheric XCO₂.

Satellite remote sensing of atmospheric XCO₂ is still in the developing stage, especially in regard to validation of satellite-derived XCO₂ products on a global scale. The principal challenge is the need for unprecedented levels of precision and accuracy to resolve long-term changes and quantify CO₂ flux; however, as an indirect observation, the accuracy of satellite detection is limited by inversion algorithms. Moreover, the validation of XCO₂ products often relies on limited *in situ* measurements. Based on prospective application in three sites, Connor et al. (2008) found

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expected errors in the OCO inverse method of less than 1×10^{-6} for all conditions. Boesch et al. (2011) found that satellite-retrieved XCO_2 is sensitive to solar zenith angle, with errors typically less than 1×10^{-6} for nadir or glint mode, but which increase to around 3×10^{-6} for the large solar zenith angles. Research has also shown that the *in situ* XCO_2 values obtained from the Total Carbon Column Observing Network (TCCON) agree well with those obtained from OCO-2, with absolute median difference of less than 0.5×10^{-6} and root mean square error (RMSE) of less than 1.5×10^{-6} (Wunch et al., 2017).

In this study, the OCO-2 XCO_2 products were comprehensively compared between *in situ* data from TCCON and Global Monitoring Division (GMD) and modeling data from CarbonTracker2019 (Dlugokencky et al., 2019; Jacobson et al., 2020). Section 2 presents the data preparation and matchup methods. Section 3 provides the comparison results and analyzes of difference among diverse data sets over the global area. Finally, the summary and conclusions are given in Section 4.

2 Data and methods

2.1 OCO-2 XCO_2 product

The OCO-2-retrieved Level-2 XCO_2 product with reprocessing version 9 from the GES-DISC platform (<http://disc.sci.gsfc.nasa.gov>) was obtained. The level-2 product provides relatively stable spatial coverage and efficient data (Liang et al., 2017). The column-averaged CO_2 dry air mole fraction XCO_2 was retrieved from the hyper-spectral radiance measured by the OCO-2. It was found that the effect of the water vapor absorption on the OCO-2 measured radiance spectra is indeed weak (Boesch et al., 2015). In addition, for the parameters relative to humidity in the XCO_2 retrieval algorithm, both the wet and dry contributions were concerned, such as the Rayleigh optical depth. This product has a spatial resolution of $2.25 \text{ km} \times 1.29 \text{ km}$ with bias correction. Quality flags are included in the product, which can assist the user in selecting high-quality data. In this study, OCO-2 XCO_2 data from January 2015 to December 2018 with a quality flag value of zero were used, corresponding to the highest quality data.

2.2 CarbonTracker modeling XCO_2 data

CarbonTracker provides four-dimensional (4-D) (i.e., time and three dimensional space) XCO_2 data. The CarbonTracker modeling data are based on global *in situ* observations of atmospheric XCO_2 and TM5 model simulation of CO_2 transportation

on the earth's surface (Peters et al., 2007). It estimates exchanges between the various carbon reservoirs, i.e., land biosphere, ocean, atmosphere, and fossil fuels. The latest CarbonTracker modeling XCO_2 data (i.e., CarbonTracker2019) were obtained from the GMD platform (<https://esrl.noaa.gov/gmd/ccgg/carbontracker>). CarbonTracker2019 provides daily global XCO_2 data and CO_2 mole fractions at 25 vertical layers with a spatial resolution of 2° (latitude) \times 3° (longitude). CarbonTracker2019 data from January 2015 to December 2018 were used (corresponding to the end date of CarbonTracker2019 at the current stage).

In terms of matchup between OCO-2 XCO_2 and CarbonTracker modeling data, the modeling data were resampled to a spatial resolution of 0.5° based on cubic spline interpolation. And then, this study matched the OCO-2 XCO_2 with the resampled modeling data based on same day and location.

2.3 TCCON *in situ* XCO_2 data

The TCCON is a global network of ground-based Fourier-transformed spectrometers that record near-infrared solar absorption spectra (Wunch et al., 2011). From these spectra, accurate and precise column-averaged abundances of CO_2 can be retrieved. The newest version of TCCON XCO_2 data were obtained from the platform (<https://tcconda.org>). TCCON provides ground-based column-averaged XCO_2 data. In this study, the column-averaged XCO_2 from 34 global TCCON sites from 2015 to 2018 were used, corresponding to the period of obtained OCO-2 XCO_2 product (Blumenstock et al., 2014; De Mazière et al., 2017; Griffith et al., 2014a, b; Hase et al., 2017; Iraci et al., 2016a, b; Kawakami et al., 2014; Kivi et al., 2014; Notholt et al., 2014, 2017; Sherlock et al., 2014a, b; Strong et al., 2017). This study used a $\pm 0.2 \text{ h}$ temporal window and 110 km spatial window to match the OCO-2-derived XCO_2 and TCCON-measured XCO_2 . Overall, total 2 473 matchups over global ocean and land were obtained, and Fig. 1 shows the distribution of TCCON sites with matchups to OCO-2-retrieved XCO_2 .

2.4 GMD *in situ* data

The GMD *in situ* CO_2 data were obtained from the NOAA-GMD platform (<https://www.esrl.noaa.gov/gmd>). The *in situ* measurement uses automated portable sampler to collect air samples. Air samples are collected approximately weekly from a globally distributed network of stations. A condenser has been added to remove a significant amount of water vapor from the sample by cooling the air stream. This change will improve the CO_2 measurements from samples collected at humid tropical loc-

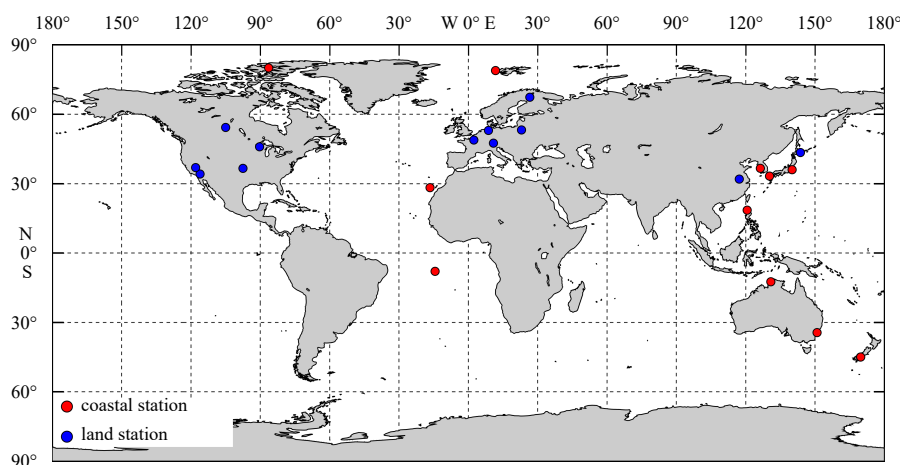


Fig. 1. Locations of the Total Carbon Column Observing Network stations with matchups to OCO-2 XCO_2 products.

ations. The *in situ* data were from 143 stations and included geographic, time, measurement details and other auxiliary information. GMD data from January 2015 to December 2018 were obtained, corresponding to the period of the obtained OCO-2 XCO₂ product. Quality control was applied in the GMD CO₂ data, and only “pass” records with rejection, selection, and information flags were used for further comparison.

It should be noted that GMD CO₂ was measured at the bottom layer of the atmosphere. To compare the OCO-2-retrieved XCO₂ column values, the GMD CO₂ data were converted to column XCO₂. The averaging kernel method was used to convert GMD measured CO₂ (XCO_{2,GMD}) to column XCO₂ (Connor et al., 2008) as:

$$XCO_{2_gmd} = XCO_{2_prior} + \sum_i^n h_i a_i (H(x) - X_a)_i,$$

where XCO_{2,prior}, a_i , and X_a represent priori, column averaging kernel, and profile values, respectively, which can all be ob-

tained from the satellite product; h is the pressure weighting function; and i is the height level. The profile of the CO₂ mole fractions (25 levels) from the CarbonTracker modeling and GMD CO₂ data was used to obtain the key parameter $H(x)$, which maps the 26 levels of CO₂ mole fractions. By combining the bottom CO₂ from GMD and vertical profile of CO₂ (25 layers) from CarbonTracker to form a 26 layer CO₂ profile, the GMD CO₂ was thus converted into column XCO₂ as measured by OCO-2.

This study used ± 5 h temporal windows to match OCO-2 and GMD XCO₂, resulting in a time difference between OCO-2 observation and GMD measurement of less than 5 h. The distance of the matchup should also be less than 100 km. It should be noted that for cases of multiple OCO-2 XCO₂ pixels matching one *in situ* sample, the average XCO₂ value for all matchup pixels was used for further comparison. Figure 2 shows the distributions of GMD stations with matchups to OCO-2 XCO₂ data. Overall, the matchup stations cover different regions of both global land and ocean, except the Antarctic.

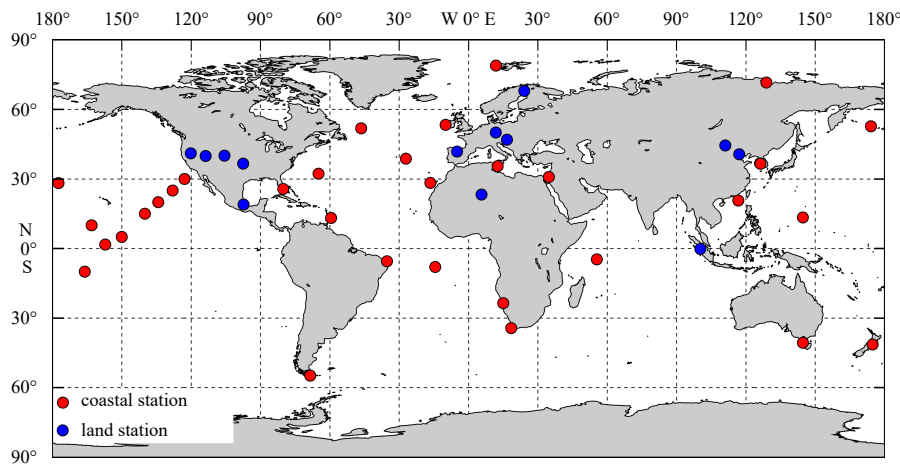


Fig. 2. Locations of the Global Monitoring Division stations with matchups to OCO-2 XCO₂ products.

3 Results and discussion

3.1 Comparisons between OCO-2 and TCCON XCO₂

Compared to the TCCON-measured XCO₂, the OCO-2 retrieved XCO₂ showed a mean absolute difference of 0.247×10^{-6} , RMSE of 1.141×10^{-6} , and correlation coefficient (R) of 0.958 for all matchups in global ocean and land, indicating good performance of the OCO-2-retrieved XCO₂ product (Fig. 3). Moreover, the OCO-2 retrieved XCO₂ showed better performance in the ocean (compared with TCCON coastal sites) than it in the land (compared with TCCON terrestrial sites), as shown in Fig. 4. Specifically, for the coastal sites, the mean absolute difference is 0.121×10^{-6} with RMSE of 1.035×10^{-6} and R of 0.965, while it is 0.412×10^{-6} with RMSE of 1.244×10^{-6} and R of 0.953 for land sites. Therefore, it is obvious that OCO-2 XCO₂ product has better consistency between satellite retrieval and *in situ* data in the oceanic region, which is expected to be related to the different retrieval algorithm and complexity of underlying surface.

Based on TCCON-measured data from 2014 to 2016, Wunch et al. (2017) found OCO-2 XCO₂ was consistent with global TCCON XCO₂ from September 2014 to April 2016, with a median difference of less than 0.5×10^{-6} , RMSE typically below 1.5×10^{-6} , and R of 0.911. Liang et al. (2017) also reported an overall bias between OCO-2 and TCCON XCO₂ of $(0.267 \pm 1.56) \times 10^{-6}$ from September 2014 to December 2016, with R of 0.879. Overall, our

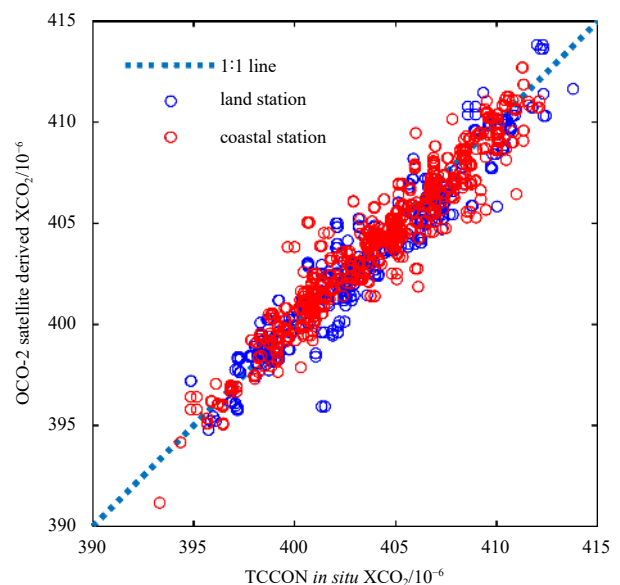


Fig. 3. Comparison between OCO-2-retrieved XCO₂ and the Total Carbon Column Observing Network (TCCON) *in situ* measurements. Red and blue points are the matchups for the oceanic and land stations, respectively. Blue dashed line represents the 1:1 line.

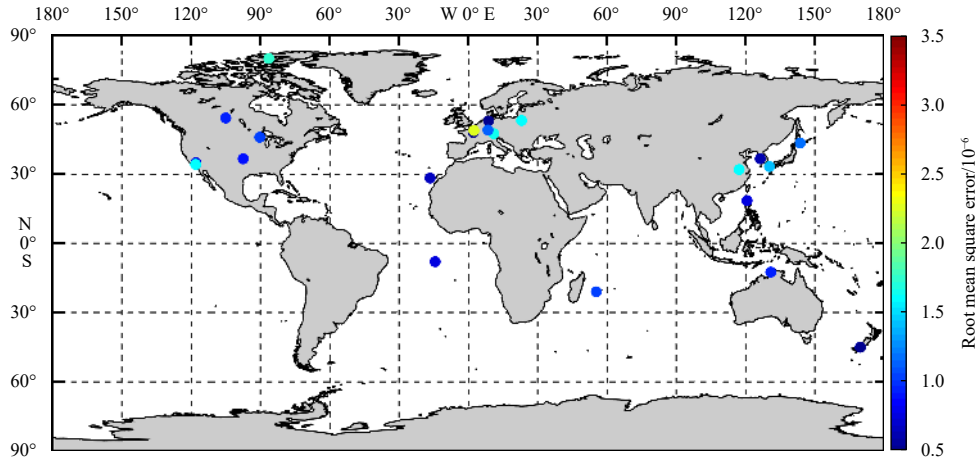


Fig. 4. The global distribution of root mean square error between OCO-2 and TCCON XCO₂ at each station.

validation results are consistent with those of previous studies, and the slight differences are likely caused by the extended period of TCCON XCO₂ from 2015 to 2018 in this study.

3.2 Comparisons between OCO-2 XCO₂ and GMD data

Figure 5 presents the comparisons between the OCO-2 and GMD XCO₂ values. Clearly, OCO-2 XCO₂ demonstrated good performance compared with GMD XCO₂, with a mean absolute difference of 0.672×10⁻⁶, RMSE of 1.684×10⁻⁶, and R of 0.865. This accuracy is comparable to the validation results between the Greenhouse Gases Observing Satellite (GOSAT) and TCCON-measured XCO₂, with a mean absolute difference of less than 0.4×10⁻⁶ (Maki et al., 2010) when considering the discrepancy between mean and mean absolute differences.

Similar to the comparison result with the TCCON XCO₂, OCO-2 XCO₂ product showed better performance over ocean (mean absolute difference of 0.441×10⁻⁶, RMSE of 1.306×10⁻⁶, and

R of 0.924) than over land (mean absolute difference of 1.372×10⁻⁶, RMSE of 2.474×10⁻⁶, and R of 0.776) as comparing with the GMD data (Fig. 6). The discrepancy between OCO-2 and GMD XCO₂ values reached 5×10⁻⁶ at some GMD stations on the land. This large discrepancy was likely due to the following reasons. First, there are several GMD stations located in complex terrains with significant spatial variability in topography or ground cover. Therefore, the low spatial resolution of the OCO-2 XCO₂ product and the matchup windows with 100 km for space and ±5 h for time may not be suitable for these stations. Although using stricter matchup windows could result in better performance, the number of effective matchups would also be reduced, making it difficult to achieve a representative assessment. Second, the modeling profiles and *in-situ* data to the OCO-2 XCO₂ observation space were mapped to estimate GMD XCO₂, which may contain some uncertainty.

It should be noted that OCO-2-retrieved XCO₂ exhibited slight overestimation at low XCO₂ and underestimation at high XCO₂ compared to the GMD XCO₂. This effect is likely caused by the different spatial resolutions between OCO-2 and GMD measurements, since OCO-2 XCO₂ is the averaged value of 2.25 km×1.29 km, while GMD XCO₂ is obtained at a specific site.

Although the matchup stations might be not large enough for the global distribution which comes from two reasons. The one is limited of XCO₂ ground-based sites, and they are mainly distributed in developed regions (usually densely populated areas). The other reason is that the satellite is along-track observation causing the low spatial resolution of the XCO₂ products.

3.3 Comparisons between OCO-2 and CarbonTracker XCO₂

Figures 7a and b show comparisons between OCO-2-retrieved and CarbonTracker-modeled XCO₂ values over land and ocean, respectively. In general, the CarbonTracker modeling results were consistent with the OCO-2-retrieved XCO₂, with R of 0.897 for land and 0.945 for ocean. Thus, the CarbonTracker XCO₂ product showed better performance over the ocean (mean absolute difference of 0.779×10⁻⁶, RMSE of 0.990×10⁻⁶) than over land (mean absolute difference of 1.023×10⁻⁶, RMSE of 1.399×10⁻⁶). The relatively larger discrepancy between CarbonTracker modeling and OCO-2 XCO₂ over land was expected to be caused by higher inhomogeneity of XCO₂ over land than over ocean. The spatial resolution of the CarbonTracker-modeled XCO₂ is rather coarse (3° in longitude and 2° in latitude). In oceanic regions, XCO₂ is relatively spatially uniform, and the effect of coarse resolution on the matchup between CarbonTracker-modeled and OCO-2-obtained XCO₂ is therefore limited. However, over land

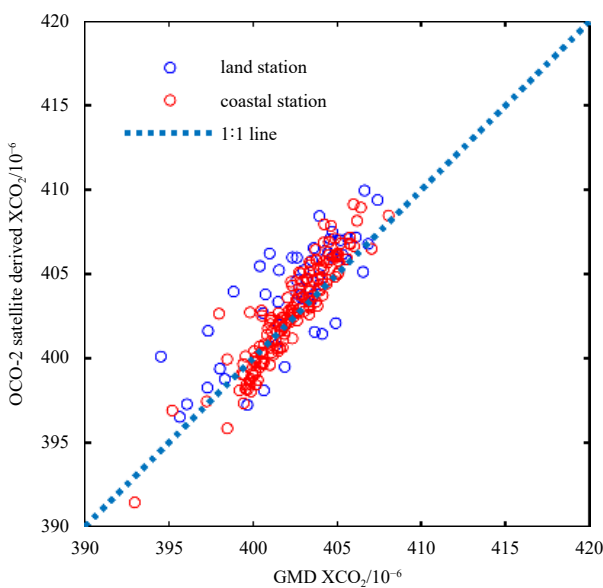


Fig. 5. The blue plots show the comparison between OCO-2-retrieved XCO₂ and the Global Monitoring Division (GMD) XCO₂ at different GMD terrestrial stations; red one for comparison between OCO-2-retrieved and GMD XCO₂ over coastal station; dashed blue line represents 1:1 line.

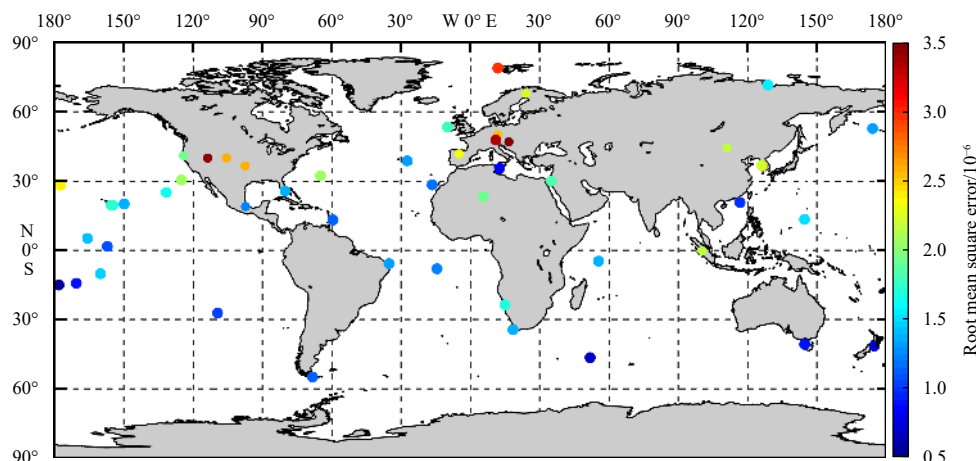


Fig. 6. The global distribution of root mean square error between GMD and OCO-2 XCO₂ at each station.

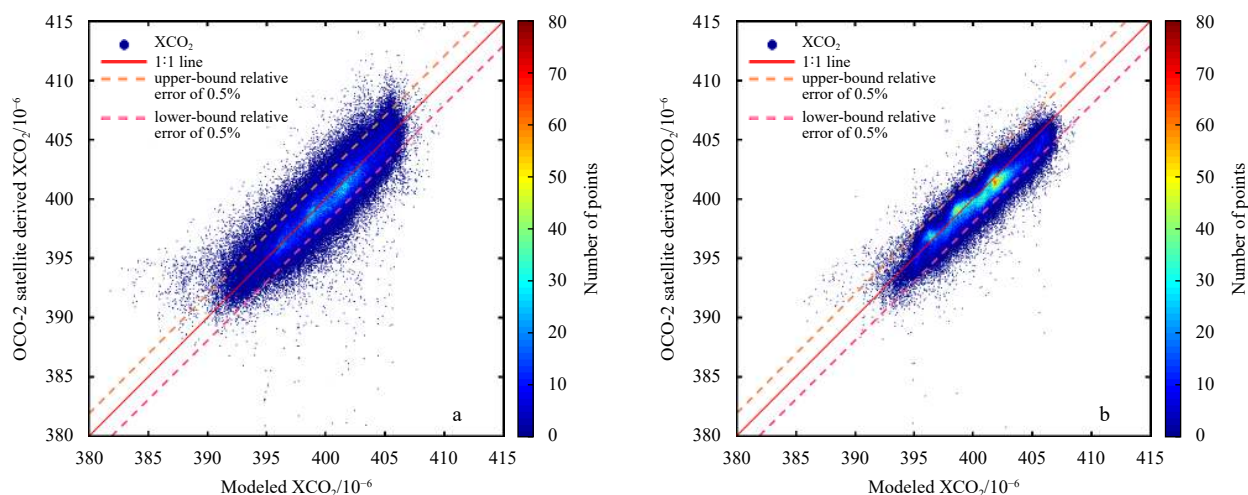


Fig. 7. Comparison between OCO-2-retrieved and CarbonTracker-modeled XCO₂. a. Comparison over land; b. comparison over ocean. Solid red line represents 1:1 line and dashed red line represents relative error of 0.5%. Color bar shows number of points.

regions, especially with high spatial inhomogeneity, the effect of coarse resolution could be significant, which might result in relatively low agreement between CarbonTracker and OCO-2 XCO₂. To quantitatively analyze the differences between OCO-2 and CarbonTracker XCO₂, their differences, i.e., $d\text{-XCO}_2$ ($d\text{-XCO}_2 = \text{XCO}_{2(\text{CarbonTracker})} - \text{XCO}_{2(\text{OCO-2})}$), were determined from 2015 to 2018. Overall, $d\text{-XCO}_2$ demonstrated near Gaussian distribution, with a mean value of -0.37×10^{-6} and standard deviation of 1.04×10^{-6} . If the matchups between two datasets were divided into two groups according to the underlying surface type (land or ocean), the mean $d\text{-XCO}_2$ for ocean was -0.17×10^{-6} (standard deviation of 0.93×10^{-6}) and for land was -0.47×10^{-6} (standard deviation of 1.18×10^{-6}).

Figure 8 showed the spatial distribution of $d\text{-XCO}_2$ at the global scale. Clearly, $d\text{-XCO}_2$ over ocean regions demonstrated obviously discrepancies between the Northern Hemisphere (NH) and Southern Hemisphere (SH). Overall, oceanic $d\text{-XCO}_2$ was higher in the NH than in the SH. When taking OCO-2 XCO₂ as a reference, the CarbonTracker-modeled XCO₂ in the NH exhibited slight underestimation over ocean regions and slight overestimation over land regions, especially in central Asia and equatorial areas. However, in the SH, the CarbonTracker XCO₂ demonstrated slight overestimation over ocean regions, except at high latitudes. If 0.3% of all points, which have the largest absolute

value of $d\text{-XCO}_2$, were extract, the underestimation of XCO₂ by CarbonTracker occurred more frequently in the mid- and low-latitude areas in the NH, especially oceanic regions, whereas the overestimation of XCO₂ by CarbonTracker occurred more often over land regions. Northcott et al. (2019) also found greatly enhanced atmospheric CO₂ levels relative to well-mixed marine atmosphere were observed during periods of offshore winds at coastal sensor platforms, which could not be exhibited by CarbonTracker.

Interestingly, there is a clear boundary for the $d\text{-XCO}_2$ in the ocean and the land. CarbonTracker uses an offline atmospheric transport model and four surface flux modules representing four crucial CO₂ transmissions. The 4-D results are interpolated for the times and locations where atmospheric observations exist, and initial net surface fluxes are adjusted using a set of weekly and regional flux scaling factors to minimize differences between the forecasted and observed CO₂ mole fractions using an ensemble Kalman filter optimization scheme with a five week lag (Williams et al., 2014). This model has certain deviations in the simulation of different underlying surfaces, and the significant gap between land and ocean does not appear to be due to a faulty gas transport model and coarse spatial resolution. These deviations are more likely from incorrect estimation of input parameters (like net ecosystem exchange) to the four surface flux

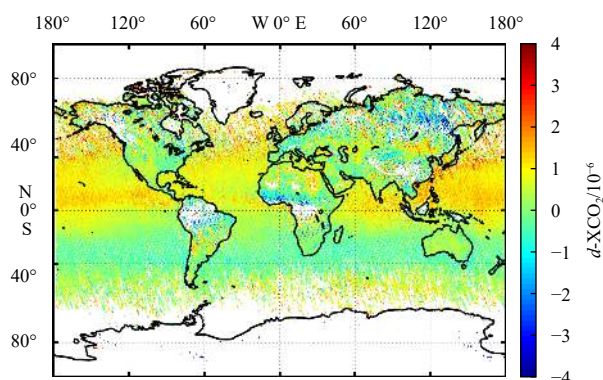


Fig. 8. Global distribution of mean differences between OCO-2 XCO_2 and CarbonTracker XCO_2 ($d-XCO_2 = XCO_{2(\text{CarbonTracker})} - XCO_{2(\text{OCO-2})}$).

modules, especially a priori net ocean surface fluxes. Although large oceanic fluxes are observed in tropical and extra-tropical oceanic regions, these values are one order of magnitude smaller than that of bio-flux emissions (Maki et al., 2010). Of course, the coarse spatial resolution of CarbonTracker may also be a possible reason why the model was unsatisfactory in simulating extreme values. In addition, the differences in the representative heights of the satellite-measured and modeled XCO_2 could induce variance between them. This effect could partly explain the underestimation and overestimation of the modeled XCO_2 over the ocean and land areas of the NH, respectively. In the ocean regions, the glint model adopted by the satellite measurement will enhance the weight of low atmosphere layers with high CO_2 , which could result in higher XCO_2 by satellite measurement. In contrast, the nadir model by satellite measurement over land will enhance the weight of upper atmosphere layers with low CO_2 , resulting in lower XCO_2 by satellite measurement.

To determine the differences in temporal variations between OCO-2 and CarbonTracker XCO_2 , the monthly average values were calculated over 2015–2018 in low-moderate latitude areas (0° – 45°) in the SH and NH, respectively (Fig. 9). Overall, the CarbonTracker-modeled XCO_2 exhibited systematically higher values than the OCO-2-derived XCO_2 in the NH, and the differences increased from 0.61×10^{-6} in 2015 to 1.28×10^{-6} in 2018, and an increase in the amplitude of seasonal XCO_2 change could be found in the high latitude areas of the NH. Some of the previously studies pointed out that these trend are primarily driven by forest expansion and increased natural vegetation growth (Forkel et al., 2016; Graven et al., 2013), while others suggested that agricultural expansion and intensification result in increased productivity and thus enhance the seasonal variations in cultivated areas at mid-latitude regions (Gray et al., 2014; Zeng et al., 2014). In the SH, the modeled data showed smaller seasonal fluctuations than the OCO-2 XCO_2 data. The SH is not considered as the main emission area of CO_2 , so it is also significance to consider the impact of different seasonal atmospheric circulation on the XCO_2 variation (Grise and Polvani, 2017). In particular, the overestimation of the modeled data showed remarkably increase from the middle of 2016 in the SH, especially in February (0.34×10^{-6} in February 2015, 0.69×10^{-6} in February 2016, 1.34×10^{-6} in February 2017, 1.32×10^{-6} in February 2018). By analyzing the February data in 2017–2018, the largest discrepancy between the modeled and OCO-2-derived XCO_2 mainly occurred in the Sahara Desert, which might be induced by uncertainty in biological flux (Williams et al., 2014).

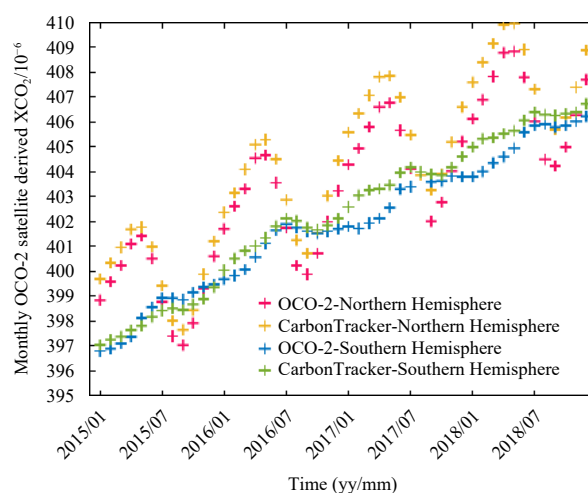


Fig. 9. Temporal variations of the monthly XCO_2 of OCO-2-derived and CarbonTracker in low-moderate latitude areas (less than 45°) in Southern Hemisphere and Northern Hemisphere from January 2015 to December 2018.

4 Conclusions

This study compared the OCO-2 XCO_2 product with *in situ* data from TCCON and GMD measurements and with CarbonTracker modeling. OCO-2 XCO_2 was consistent with TCCON-measured XCO_2 , with a mean absolute difference of 0.247×10^{-6} and RMSE of 1.141×10^{-6} . Compared with the GMD-derived XCO_2 , the OCO-2-retrieved XCO_2 had a mean absolute difference of 0.672×10^{-6} and RMSE of 1.684×10^{-6} . These high agreements showed that the OCO-2 could provide high quality XCO_2 data over the low-moderate latitude regions. Moreover, the comparison between satellite and modeling product showed that they were relatively consistent with each other, with a mean absolute difference of 1.02×10^{-6} over land and 0.78×10^{-6} over ocean. In addition, the comparison results showed that the agreement among three different types dataset of XCO_2 was higher in the oceanic area than it in the terrestrial area, indicating the high applicable of the OCO-2-retrieved XCO_2 product to estimate the air-sea CO_2 flux over ocean. Our results also evidenced the reliable of the CarbonTracker modeling XCO_2 data, and with the advantage of the global coverage, this modeling data can also be used to estimate the air-sea CO_2 flux over ocean when satellite product is unavailable.

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