Validation of GOSAT SWIR XCO$_2$ and XCH$_4$ Retrieved by PPDF-S Method and Comparison with Full Physics Method

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Abstract

Column-averaged concentrations of carbon dioxide (XCO$_2$) and methane (XCH$_4$) were retrieved from spectra observed by the Greenhouse gases Observing SATellite (GOSAT) using the so-called Photon path length Probability Density Function-Simultaneous (PPDF-S) retrieval method, which explains cloud/aerosol effects in terms of light path modification. The PPDF-S data, as well as the standard products for General Users (GU) of XCO$_2$ and XCH$_4$ retrieved using the full physics (FP) method, were validated through comparison with Total Carbon Column Observing Network (TCCON) data. Results show that bias and its standard deviation of XCO$_2$ over the land are 0.73 and 1.83 ppm for the PPDF-S data, and −0.32 and 2.16 ppm for GU products. For XCH$_4$, they are 1.4 and 14.1 ppb, and −1.9 and 12.5 ppb, respectively. Although the magnitude relations between XCO$_2$ and XCH$_4$ retrieved by the PPDF-S and GU products are identical over the land, they differ over the ocean. This fact emphasizes the importance of additional validation data over the ocean. Results also show that 68% of FP data that were screened out through an Aerosol Optical Thickness (AOT) test passed all screening tests for the PPDF-S method, implying the applicability of the PPDF-S method to denser aerosol conditions.

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1. Introduction

Because of human activity, atmospheric concentrations of carbon dioxide (CO$_2$) and methane (CH$_4$) have increased since the Industrial Revolution. To estimate sources and sinks of CO$_2$ and CH$_4$, the Greenhouse gases Observing SATellite (GOSAT) was launched in 2009. It measures backscattered sunlight by the surface or atmosphere of the earth in Short-Wavelength InfraRed (SWIR) with near-global coverage. Column-averaged concentrations of carbon dioxide (XCO$_2$) and methane (XCH$_4$) can be retrieved from the measured spectra.

Satellite-retrieved XCO$_2$ and XCH$_4$ tend to show some biases, mainly attributable to light scattering by clouds and aerosols. In the Full Physics (FP) retrieval method that is used widely for gas retrieval, the multiple light scattering processes are calculated explicitly by solving radiative transfer equations accounting for optical properties of aerosols under a clear sky condition (Morino et al. 2011; Yoshida et al. 2011, 2013).

A more simplified estimation method, a photon path length probability density function (PPDF)-based method, has been proposed (e.g., Bril et al. 2007; Oshchepkov et al. 2008, 2009, 2013). The method can represent the effects of non-negligible light path modification without exact radiative transfer simulations because the light path modification is evaluated using PPDF statistically. In the new version of the PPDF-based method, the PPDF-simultaneous (PPDF-S) method, gas concentrations are retrieved simultaneously with PPDF parameters and its retrieval uncertainty for GOSAT was evaluated (Oshchepkov et al. 2013). However, because evaluation was made only for XCO$_2$ and because the data period was limited, further validation is necessary.

The objective of this study is to clarify the uncertainty and global characteristics of PPDF-S retrieval results for both XCO$_2$ and XCH$_4$ for an extended data period through comparison of them with ground-based Total Carbon Column Observing Network (TCCON) data that are generally used as reference for satellite measurements (Wunch et al. 2011a; Blumenstock et al. 2014; Wunch et al. 2015). For comparison, we also analyzed data of XCO$_2$ and XCH$_4$ retrieved using the FP method and released by the National Institute for Environmental Studies (NIES).

2. GOSAT retrieval method and data used for this study

2.1 PPDF-S method

The PPDF data reflect statistical characteristics of the photon path length. Using two equations, the radiance, as affected by scattering and absorption in a homogeneous medium $I(k)$, can be represented as the radiance observed at an absorption-free wavelength that is close to the absorption band $I_0 = I(k = 0)$ and PPDF.

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$$I(k) = I_0 T(k) = I_0 \int_0^\infty \exp(\quad kL)P(L)dL$$

$$\int_0^\infty P(L)dL = 1,$$

where, T is transmittance, L the photon path length, k the volume absorption coefficient, and $P(L)$ denotes the PPDF with respect to the photon geometrical path (Bennartz and Preusker 2006).

According to Bril et al. (2007), the equations above are applicable for retrieving greenhouse gas concentration from satellite observational data. Herein, PPDF is explained using PPDF parameters accounting for single light scattering by a cloud/aerosol layer as well as multiple light scattering/reflection between the layer and the ground surface. Oshchepkov et al. (2009) pointed out that the PPDF can be represented by four PPDF parameters: the altitude of the cloud/aerosol layer h; the relative reflection of the cloud/aerosol layer α, which represents the relative fraction of the photons scattered singly to the detector; ρ, which characterizes the relative mean path length between the layer and ground surface; and an adjustment parameter γ accounting for multiple scattering/reflection.

Oshchepkov et al. (2013) investigated the uncertainty of XCO_2 retrieved using the PPDF-S method (hereinafter called PPDF-S data) for June 2009 through July 2010. The present study evaluated both XCO_2 and XCH_4 retrieved using the PPDF-S method from the spectral radiance products labeled as V161.160 for June 2009 through May 2014. Hereinafter, we use labeling names, Level 1B (L1B) and Level 2 (L2), respectively for spectral radiance and XCO_2 and XCH_4.

2.2 NIES standard products

NIES releases the L2 data as the standard products for General Users (i.e., GU products) retrieved using FP method, which is widely used for gas retrieval (Yoshida et al. 2011, 2013). Morino et al. (2011) reported the uncertainty of GU products derived from April 2009 through October 2009 by comparing them with TCCON data. Yoshida et al. (2013) validated GU products in the same way for a longer period of June 2009 through July 2010, but the version of L1B data used for retrieval is a mix of V141.141, V150.150, and V150.151. We used a later version of GU products

than those used by Yoshida et al. (2013), which were retrieved from L1B in V161.160 for June 2009 through May 2014. They are labeled as V02.21 of the L2 data. We also used the L2 data released only for Research Announcement principal investigators (RA products). Differences between GU products and RA products are just criteria for data screening tests applied to control the data quality. The GU products are selected from RA products using seven screening tests with thresholds of four parameters (e.g., aerosol optical thickness), which means that the screening criteria for GU products are stricter than those for RA products (Yoshida et al. 2011, 2013). The numbers of observational scenes used in this study are 494,259 and 878,762, respectively, for GU and RA products.

2.3 TCCON data and validation methodology

The TCCON is a global network of ground-based Fourier Transform Spectrometers (FTS) measuring the solar spectrum in the near-infrared almost continuously under a clear sky condition, to retrieve column abundances of CO_2, CO, CH_4, N_2O and other molecules (Wunch et al. 2011a). Although the observational principles of TCCON and GOSAT are similar, TCCON measures the direct solar spectrum with higher spectral resolution and better calibrated. Accordingly, TCCON data have been used to validate GOSAT data because they are more reliable than those obtained from satellite measurements.

For this study, we used TCCON data from 11 sites presented in Table 1. An open source software package (GGG) is used to calculate total column abundances of the gases from measured spectra. TCCON data analyzed using the GGG2009 and GGG2012 version of retrieval algorithm were used respectively by Morino et al. (2011) and by Yoshida et al. (2013). For this study, we used data analyzed using the newest version of the algorithm: GGG2014.

To validate GOSAT data using TCCON data, GOSAT data within a 4×4 degree grid box centered at each TCCON site and TCCON data measured within $\pm$ 30 min of GOSAT overpass time were selected. To represent the GOSAT data uncertainty, we define the three parameters presented below.
- *diff*.: (GOSAT data) – (TCCON data)
- *B*: mean value of *diff*.
- σ: standard deviation of *diff*.

Table 1. TCCON sites used for this study.

Site	Latitude	Longitude	Dataset reference	TCC0N software version and release number
Bialystok	53.23 N,	23.03 E	Deutscher et al., 2015. doi:10.14291/tccon.ggg2014.bialystok01.R1/1183984.	GGG2014.R1
Bremen	53.10 N,	8.85 E	Notholt et al., 2014. doi:10.14291/tccon.ggg2014.bremen01.R0/1149275.	GGG2014.R0
Garmisch	47.48 N,	11.06 E	Sussmann et al., 2014. doi:10.14291/tccon.ggg2014.garmisch01.R0/1149299.	GGG2014.R0
Orléans	47.97 N,	2.11 E	Warneke et al., 2014. doi:10.14291/tccon.ggg2014.orleans01.R0/1149276.	GGG2014.R0
Lamont	36.60 N,	97.49 W	Wennberg et al., 2016. doi:10.14 291/tccon.ggg2014.lamont01.R1/1255070.	GGG2014.R1
Park Falls	67.37 N,	90.27 W	Wennberg et al., 2014. doi:10.14291/tccon.ggg2014.parkfalls01.R0/1149161.	GGG2014.R0
Sodankylä	67.37 N,	26.63 E	Kivi et al., 2014. doi:10.14291/tccon.ggg2014.sodankyla01.R0/1149280.	GGG2014.R0
Tsukuba125HR	36.05 N,	140.12 E	Morino et al., 2016. doi:10.14291/tccon.ggg2014.tsukuba02.R1/1241486.	GGG2014.R1
Darwin	12.43 S,	130.89 E	Griffith et al., 2014a. doi:10.14291/tccon.ggg2014.darwin01.R0/1149290.	GGG2014.R0
Lauder125HR	45.05 S,	169.68 E	Sherlock et al., 2014. doi:10.14291/tccon.ggg2014.lauder02.R0/1149298.	GGG2014.R0
Wollongong	34.41 S,	150.88 E	Griffith et al., 2014b. doi:10.14291/tccon.ggg2014.wollongong01.R0/1149291.	GGG2014.R0

Generally, when column-averaged gas concentrations observed using instruments of different types are compared, differences in a priori profiles assumed in analyses and the column averaging kernels, which represent the sensitivity profiles, should be considered. Although Wunch et al. (2011b) reported that the bias in XCO_2 attributed to the differences in a priori and averaging kernel is about 0.6 ppm for GOSAT data at a TCCON site (Lamont, CA, USA), we do not consider the differences in this study so as to make our validation method to be same as that of an earlier study by Yoshida et al. (2013).

3. Results

3.1 Validation results of global data

Figures 1a and 1b respectively depict global maps of XCO_2 and XCH_4 of PPDF-S data and GU products. All global maps in this paper describe the mean value in a grid of 2.5×2.5 degree box for the whole data period of June 2009 − May 2014. The most distinctive difference over land between PPDF-S data and GU

products is found over the middle of Africa, where biomass burning often occurs and where many aerosols exist. In this region, the PPDF-S data have lower XCO_2 and XCH_4 than GU products, but there are no TCCON data available for validation.

To investigate the temporal variation of biases, time series of monthly biases of PPDF-S data and GU products and their standard deviations averaged over the 11 TCCON sites are presented in Fig. 2. The biases are not uniform during the operational period. Moreover, the temporal features in the variabilities are not the same for XCO_2 and XCH_4. The bias of XCO_2 of GU products has a larger negative bias in 2009 and 2010, which then decreased to zero around 2011 until 2014. However, the XCH_4 of PPDF-S data has a positive bias in 2009 and 2010. In later analyses, we shall present validation results separately for 2009−2010 and 2011−2014.

Tables 2 and 3 present the validation results obtained using TCCON data observed at 11 sites from June 2009 through May 2014. Table 2 shows the difference in uncertainty of PPDF-S data and GU products. Results for 2009−2010 (data period (1)) and for 2011−2014 (data period (2)) are also presented separately in the
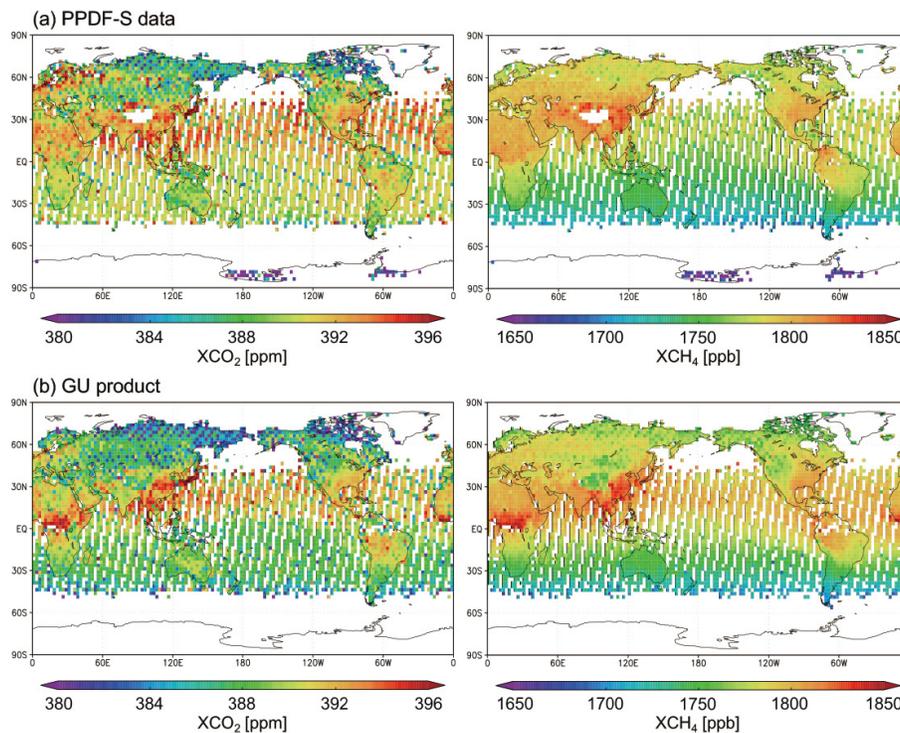

Fig. 1. (a) Global maps of the mean value of XCO_2 (left) and XCH_4 (right) in a grid of 2.5×2.5 degree box for the whole data period of June 2009−May 2014 for PPDF-S data: (b) as in (a), but for GU products.
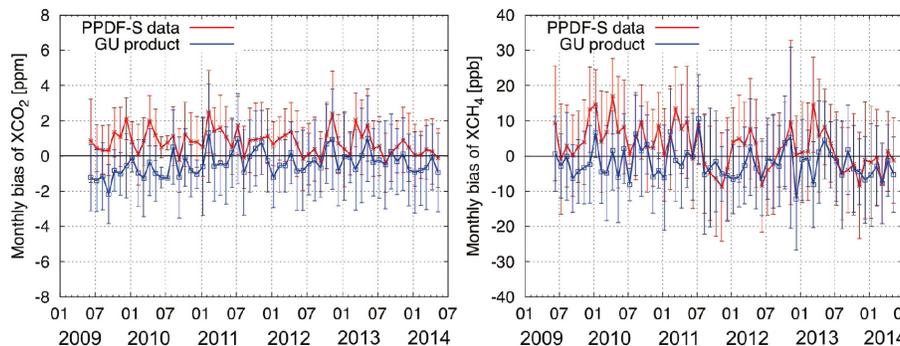

Fig. 2. Time series of monthly biases of PPDF-S data (red line) and GU products (blue line) and its deviations: the left panel is for XCO_2; the right one is for XCH_4.

Table 2. Validation results evaluated using TCCON data observed at 11 sites during June 2009−May 2014 for common cases between PPDF-S data and GU products: N, number of data; B, bias; σ, standard deviation.

| | | XCO$_2$ | | | | XCH$_4$ | | | |
| | | PPDF-S data | | GU product | | PPDF-S data | | GU product | |
Site	N	B [ppm]	σ [ppm]	B [ppm]	σ [ppm]	B [ppb]	σ [ppb]	B [ppb]	σ [ppb]
Bialystok	58	1.6	1.63	0.26	1.96	4.1	10.6	1.7	10.5
Bremen	36	2.05	1.56	0.57	1.50	−2.5	14.1	−1.3	9.1
Garmisch	94	1.39	1.77	0.01	2.19	4.7	14.0	3.3	15.4
Orléans	199	0.81	1.40	−0.54	1.82	−3.6	13.1	−3.4	10.5
Lamont	598	0.42	1.63	−1.42	1.68	5.5	12.4	−4.4	11.5
Park Falls	173	0.83	1.89	−0.07	1.91	4.0	13.1	3.7	10.0
Sodankylä	49	1.68	1.50	0.59	1.65	3.8	9.8	1.2	9.3
Tsukuba	277	1.76	2.05	1.66	2.14	−1.3	14.4	3.7	11.8
Darwin	150	−0.52	1.38	−0.73	1.64	−14.5	8.7	−4.5	7.6
Lauder	132	0.34	1.25	−0.35	1.18	8.8	11.0	−1.7	8.2
Wollongong	352	0.47	1.96	−0.25	2.51	1.0	15.0	−5.3	16.0
Total	2118	0.73	1.83	−0.32	2.16	1.4	14.1	−1.9	12.5
(1) 2009−2010	404	0.95	1.70	−0.76	1.86	5.6	13.2	−0.8	11.3
(2) 2011−2014	1714	0.68	1.86	−0.22	2.22	0.4	14.2	−2.2	12.7

Table 3. Averaged validation results obtained using TCCON data observed at 11 sites for all cases of PPDF-S data and GU products for the whole data period: N, B and σ are the same as in Table 2; r is the correlation coefficient between collocated GOSAT and TCCON data; a is the slope of the regression line.

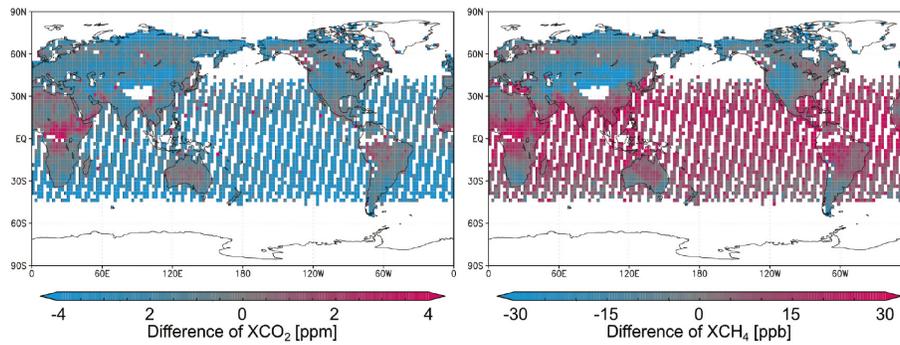| | | XCO$_2$ | | | | XCH$_4$ | | | |
	N	B [ppm]	σ [ppm]	r	a	B [ppb]	σ [ppb]	r	a
All PPDF-S data	2804	0.47	2.09	0.89	0.96	0.66	15.41	0.87	0.95
All GU product	2895	−0.29	2.33	0.88	0.99	−2.24	13.14	0.91	0.99

Fig. 3. Differences in XCO$_2$ (left) and XCH$_4$ (right) between PPDF-S data and GU products that are calculated using subtracting PPDF-S data from the GU products. Values are averages over the whole data period in a grid of 2.5 × 2.5 degree box.

table. Table 3 shows the results for all cases of PPDF-S data and GU products obtained for the whole data period: N is the number of data; B represents the bias (in units of parts per million (ppm) for XCO$_2$ and parts per billion (ppb) for XCH$_4$); σ is the standard deviation (in the same units as B); r is the correlation coefficient between collocated GOSAT and TCCON data; and a denotes the slope of the regression line. Results show that the orders of the bias are similar between PPDF-S data and GU products, but B of PPDF-S data is positive, whereas that of GU products is negative. Furthermore, XCO$_2$ of both PPDF-S data and GU products have larger absolute values of B and smaller σ in period (1) than those in period (2), as depicted in Table 2. Actually, XCH$_4$ of both PPDF-S data and GU products have larger σ in (2) than those in (1), but the absolute value of B is extremely large for PPDF-S data in (1) and for GU products in (2). Among the 11 TCCON site data, B of XCO$_2$ for PPDF-S data at Darwin is negative. This point will

be discussed in Section 4.

To illustrate the spatial distribution of the difference between PPDF-S data and GU products, we present a global map of the difference between the two products in Fig. 3 by subtracting PPDF-S data from GU products. Differences over land show similar features between XCO$_2$ and XCH$_4$. However, XCO$_2$ of PPDF-S data are larger and XCH$_4$ of PPDF-S data are smaller over the ocean compared to GU products.

3.2 Validation results under large AOT conditions

An important parameter used in screening tests for selecting GU products from RA products is the aerosol optical thickness (AOT). For the whole data period in this paper, 211 cases of RA product for which AOT is evaluated as larger than 0.1 are excluded to produce GU product. The value of AOT is retrieved simultaneously with gas concentration in the FP method, assuming other

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Table 4. Validation results evaluated using TCCON data observed at 11 sites for the excluded RA product through the AOT screening test and PPDF-S data for the comparable scenes: N, B and σ are the same as in Table 2.

XCO_2	RA product screened out through the AOT test			corresponding PPDF-S data for the comparable scenes		
	N	B [ppm]	σ [ppm]	N	B [ppm]	σ [ppm]
(1) 2009−2010	73	−1.57	2.68	58	1.00	1.45
(2) 2011−2014	138	−1.12	3.74	86	−0.14	1.85
2009−2014	211	−1.27	3.03	144	0.32	1.47

XCH_4	N	B [ppb]	σ [ppb]	N	B [ppb]	σ [ppb]
(1) 2009−2010	73	6.6	13.2	58	16.6	10.0
(2) 2011−2014	138	0.2	17.5	86	3.3	12.5
2009−2014	211	2.4	14.2	144	8.7	10.5

optical parameters of aerosols (Yoshida et al. 2011).

To investigate the uncertainty of GOSAT data with large AOT, we used AOT estimated in the FP method as a measure of the aerosol concentration, and compared data removed from RA products through the AOT test with the PPDF-S data for the same cases. Table 4 presents results for 2009−2010, 2011−2014, and 2009−2014. The results for 2009−2014 showed that 144 observational scenes (= 68%) out of the 211 scenes passed all the PPDF-S screening tests. When the 144 cases are validated with the TCCON data, both B and σ of XCO_2 of the PPDF-S data is smaller than that of the removed RA products. Contrary to the results of XCO_2, B of XCH_4 of the PPDF-S is larger than that of the RA products.

4. Discussion

From the validation results shown in Tables 2 and 3, the magnitudes of B and σ were found to be almost identical between PPDF-S data and GU products. Therefore, it can be inferred that PPDF-S data have some potential for use in source–sink inversion analyses of gases as well as GU products after appropriate bias correction, as far as σ does not change so much after bias correction. Results also show that the characteristics of the biases have changed since 2010, as depicted in Fig. 2 and Table 2. This change might result from changes in the spectral radiance characteristics. This point should be investigated further in future studies.

As shown in Table 2, B of XCO_2 of PPDF-S data is negative only at Darwin, which is the only site where collocated GOSAT data were observed over the ocean. This negativity implies that XCO_2 observed over the ocean and analyzed by the PPDF-S method has generally negative B. Furthermore, as portrayed in Fig. 3, large differences exist in both XCO_2 and XCH_4 between PPDF-S data and GU products over the ocean. The difference of XCH_4 can be as great as 20 ppb. Saitoh et al. (2012) compared the XCH_4 of GU product with aircraft data and reported that the difference was −8 ppb with the standard deviation of 10 ppb; XCH_4 of PPDF-S data might have larger biases compared with GU products over the ocean. It is important to validate the GOSAT data over the ocean to ensure the global characteristics of the GOSAT data. However, GOSAT data over the ocean have not been validated sufficiently in this study because TCCON data were measured on the land. It is necessary to increase the number of validation data over the ocean to ensure the uncertainty of GOSAT ocean data.

Although the validation results presented in Table 4 show that the PPDF-S method exhibits better performance than the FP method to retrieve XCO_2 under high AOT conditions, it is difficult to clearly discern which method is more advantageous for retrieving gas concentrations under high aerosol conditions

because relations between the estimated AOT and actual aerosol conditions have not been well studied. It is important to evaluate the characteristics of PPDF-S method through direct comparison with aerosol concentrations or AOT values observed independently from GOSAT measurements. Another means of investigating the retrieval method performance is a simulation study assuming various aerosol conditions in the atmosphere (Aben et al. 2007; Butz et al. 2009). Sensitivities of aerosol parameters to the retrieval accuracy should be examined through simulations conducted in future studies.

5. Summary and concluding remarks

XCO_2 and XCH_4 retrieved using the PPDF-S method and GU products have been validated using TCCON data at 11 sites. The uncertainties of PPDF-S data and GU products, defined as B and σ, are almost equal for both XCO_2 and XCH_4. Actually, PPDF-S data have positive B in both XCO_2 and XCH_4. By contrast, GU products show negative B. The biases also show temporal variation during 2009−2014, with changing characteristics of the biases since 2010.

We found large differences in both XCO_2 and XCH_4 between PPDF-S data and GU products over the ocean. It is necessary to increase the number of validation data to assess the uncertainty of GOSAT data over the ocean. At the same time, PPDF-S data have smaller values of both XCO_2 and XCH_4 than those of GU products, particularly over the middle of Africa, where many aerosols might exist because of biomass burning.

GU products were selected from RA products using some screening tests. B and σ of XCO_2 of PPDF-S data are smaller than those of the data removed from RA products through the AOT test for the comparable observational scenes. From results of this analysis, we inferred that PPDF-S and FP methods exhibit different performance under high-AOT conditions implying the applicability of the PPDF-S method to denser aerosol conditions. To ascertain which method is superior under high aerosol conditions, simulation studies or validation using aerosol measurements are necessary for future researches.

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