



Update on the GOSAT TANSO–FTS SWIR Level 2 retrieval algorithm

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Abstract. The National Institute for Environmental Studies has provided the column-averaged dry-air mole fraction of carbon dioxide and methane (XCO₂ and XCH₄) products (L2 products) obtained from the Greenhouse gases Observing SATellite for more than a decade. Recently, we updated the retrieval algorithm used to produce the new L2 product, V03.00. The main changes from the previous version (V02) of the retrieval algorithm are the treatment of cirrus clouds, the degradation model of the Thermal And Near-infrared Spectrometer for carbon Observation – Fourier Transform Spectrometer (TANSO-FTS), solar irradiance spectra, and gas absorption coefficient tables. The retrieval results from the updated algorithm showed improvements in fitting accuracies in the O₂ A, weak CO₂, and CH₄ bands of TANSO-FTS, although the residuals increase in the strong CO₂ band over the ocean. The direct comparison of the new product obtained from the updated (V03) algorithm with the previous version V02.90/91 and the validations using the Total Carbon Column Observing Network revealed that the V03 algorithm increases the amount of data without diminishing the data qualities of XCO₂ and XCH₄ over land. Further, the negative bias of XCO₂ is larger than that of the previous version over the ocean, and bias correction is still necessary. Additionally, the V03 algorithm resolves the underestimation of the XCO₂ growth rate compared with the in situ measurements over the ocean recently found using V02.90/91 and V02.95/96.



35 1 Introduction

The Greenhouse gases Observing SATellite (GOSAT) is the joint project of the Japan Aerospace Exploration Agency, the Ministry of the Environment, and the National Institute for Environmental Studies (NIES), and is the first satellite dedicated to monitoring greenhouse gases (GHGs), such as carbon dioxide (CO₂) and methane (CH₄) from space (Yokota et al., 2009). Since its launch on January 23, 2009, it has constantly provided the global concentrations of GHGs for more than 13 years. Additionally, the successor of GOSAT, GOSAT-2 was launched in 2018 and is also still in orbit. The sensor onboard GOSAT, Thermal And Near-infrared Sensor for carbon Observation (TANSO) consists of two instruments, the Fourier Transform Spectrometer (FTS; Kuze et al., 2009) and the Cloud and Aerosol Imager (CAI). TANSO-FTS measures the spectral regions ranging as 0.758–0.775 μm (12,900–13,200 cm⁻¹), 1.56–1.72 μm (5,800–6,400 cm⁻¹), and 1.92–2.08 μm (4,800–5,200 cm⁻¹) in short-wavelength infrared (SWIR) and 5.56–14.3 μm (700–1,800 cm⁻¹) in the thermal infrared (TIR) regions, with a spectral interval of approximately 0.2 cm⁻¹ and a spectral resolution (defined as the full width at half maximum of the instrumental line shape function) of 0.262 – 0.367 cm⁻¹ in the SWIR bands (Kuze et al., 2009). The trace gas concentrations or cloud properties have been estimated from the SWIR bands (Yoshida et al., 2011; 2013) and the TIR band (Saitoh et al., 2009; 2016; Ohyama et al., 2012; Someya et al., 2016; 2020).

The SWIR bands measure the reflected sunlight to estimate column-averaged dry-air mole fractions of CO₂ (XCO₂) and CH₄ (XCH₄). NIES provides the SWIR Level 2 (L2) product, which contains XCO₂ and XCH₄ retrieved using the GOSAT SWIR spectra (Yoshida et al., 2011; Yoshida et al., 2013). The L2 product is used to estimate the global surface fluxes of CO₂ and CH₄ and the resulting concentration distributions provided as Level 4 products (Maksyutov et al., 2013). Other groups have developed retrieval algorithms for GOSAT and provided column-averaged dry-air mole fractions of CO₂ and CH₄ (Butz et al., 2011; Parker et al., 2011; Oshchepkov et al., 2011; O'Dell et al., 2012; Cogan et al., 2012; Kikuchi et al., 2016; Noël et al., 2021). The major differences among these algorithms include, e.g., the treatments of atmospheric particles or radiative transfer calculations. The algorithms are roughly classified into two categories considering whether multiple scattering by clouds and aerosols which are critical sources of error is explicitly considered, or not.

The current version of the NIES SWIR L2 product is the version 02 series (V02.xx), which has been improved from the previous version in several ways such as the treatment of the aerosols (Yoshida et al., 2013). Owing to this improvement, both the biases and precisions against the ground-based measurements, the Total Carbon Column Observing Network (TCCON; Wunch et al., 2011), are much less than 1% for XCO₂ and XCH₄. However, the systematic structures in the spectral residuals still exist in the retrieval results, and the increase of data amount in the L2 product is further required. In addition, inconsistencies in the annual CO₂ growth rate compared with the in situ measurements were recently found in the V02.90/91 and V02.95/96 products. Therefore, the retrieval algorithm was updated to V03 to address these issues. Herein, we present an algorithm for the new version of the NIES SWIR L2 product, V03.xx.



2 Current retrieval algorithm

2.1 NIES V02 retrieval algorithm

The retrieval algorithm for the SWIR L2 product developed at NIES (Yoshida et al., 2013) is a full physics-based algorithm, that explicitly considers the scattering processes by particles in the atmosphere in the radiative transfer calculation. Four spectral ranges, 12,950–13,200 cm⁻¹ (O₂ A sub-band), 6,180–6,380 cm⁻¹ (WCO₂ sub-band), 5,900–6,150 cm⁻¹ (CH₄ sub-band), and 4,800–4,900 cm⁻¹ (SCO₂ sub-band) are used for the retrievals. The retrieval algorithm is based on the maximum a posteriori solution (Rodgers, 2000). This method obtains a solution to the state by minimizing the cost function,

$$J(\mathbf{x}) = [\mathbf{y} - \mathbf{F}(\mathbf{x}, \mathbf{b})]^T \mathbf{S}_\epsilon^{-1} [\mathbf{y} - \mathbf{F}(\mathbf{x}, \mathbf{b})] + (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_a)$$

where \mathbf{y} represents the measurement vector, \mathbf{F} denotes a forward model, \mathbf{x} is a state vector, \mathbf{b} denotes a model parameter vector, \mathbf{S}_ϵ represents a measurement error covariance matrix, \mathbf{x}_a denotes an a priori state vector, and \mathbf{S}_a represents an a priori covariance matrix. In the NIES retrieval algorithm, the state vector contains the profiles of the gases (CO₂, CH₄, and H₂O) and two types of aerosols, surface albedo over land, wind speed over the ocean surface, surface pressure (Ps), vertically constant temperature shift, zero level offset for the O₂ A sub-band, and wavenumber dispersions for each sub-band. The a priori values of CO₂ and CH₄ are obtained from the NIES transport model (NIES-TM; Saeki et al., 2013), and those of aerosol concentrations are from the Spectral Radiation-Transport Model for Aerosol Species (SPRINTARS; Takemura et al., 2000). Meteorological information is taken from the grid point value (GPV) objective analysis data using the global spectral model (GSM) provided by the Japanese Meteorological Agency. The atmosphere is divided into 15 vertical layers for radiative transfer calculations; the gas optical thickness is calculated every 12 sub-layers in each layer, i.e., 180 sub-layers in total.

2.2 Motivation for algorithm update

Although the number of TANSOFTS observations in the daytime is approximately 9000 per day, less than 10% of the total observations pass through the cloud screening and quality control filters to produce the L2 product. Thus, increasing the available number of observations for the L2 product is desirable to increase the TANSO-FTS measurement coverage. The existence of clouds is the main reason for the decrease in the available number of observations. The V02 algorithm discriminates the cloudy scenes using CAI images and the water vapor saturation band near 2 μm, which are mainly used to discriminate optically thick and cirrus clouds, respectively (Yoshida et al., 2011). In the V03 algorithm, cirrus cloud screening using the water vapor saturation band is not applied. Instead, we attempt to retrieve cirrus clouds simultaneously with the GHGs to increase the number of observations.

The spectral residuals obtained from the V02 retrievals have systematic wavenumber-dependent structures. The main causes of these structures are the uncertainties of the solar irradiance spectra and spectroscopic parameters of the trace gases. These datasets are updated to reduce the systematic residuals. In addition, the common use of these datasets with the



GOSAT-2 retrievals makes the L2 product from both satellites homogeneous. The homogeneousness of the products makes their continuous and simultaneous use easy.

100 According to the validation study, biases in the retrieval results of XCO₂ and XCH₄ without bias correction indicate spatial and temporal dependencies, significantly affecting the flux inversions and production of the Level 4 products. Therefore, NIES provides the bias-corrected product (V02.95/96) as well as the bias-uncorrected one (V02.90/91). Recently, we found that the growth rate of the XCO₂ estimated from the GOSAT L2 product, V02.95/96 or V02.90/91 over the ocean is lower than that over land, or the validation data such as TCCON and in situ measurements (NIES GOSAT project, 2021). Due to this issue, the GOSAT L2 V02.97/98 product with additional correction applied to its long-term trend based on the bias-
105 corrected V02.95/96 product, has been released. The sensitivity degradation of TANSO-FTS could be the main cause of this issue. In this study, the degradation model is updated to decrease the temporal dependencies.

3 Updates on the retrieval algorithm

3.1 Treatment of cirrus clouds

110 The 2 μm band cloud screening mentioned in Section 2.2 is not performed in the V03 algorithm. Alternatively, the spectral band, 5150 to 5200 cm⁻¹ (H₂O sub-band) is additionally used in the retrieval to simultaneously estimate the cloud optical thickness (COT) and cloud top pressure (CTP) with GHG concentrations. We assume a single cloud layer with a pressure thickness of 30 hPa in which the ice particles with an effective dimension of 20 μm are homogeneously distributed. The optical property of the ice particle is obtained from the generalized habit mixture model proposed by Baum et al., (2011). The a priori values of COT and CTP are 0.1 and 150 hPa globally. If the retrieved COT is larger than 0.1, the post-screening
115 process rejects the observation.

3.2 Degradation model

The radiometric sensitivity of TANSO-FTS has been degraded exponentially as a function of time relative to the pre-launch calibration with spectral dependencies. The V02 algorithm considers this degradation based on the degradation model developed by Yoshida et al. (2012). The V03 algorithm employs the model recently developed by Someya and Yoshida
120 (2020). This model was constructed from the temporal variations of the principal components obtained from on-orbit solar irradiance calibration data using a diffuser plate to distinguish and separately evaluate the components. Although the new degradation model used in V03 and the previous one used in V02 are usually similar, the differences were found with several spectral dependencies. These differences increase with time because the new degradation model was constructed based on the longer data period. Therefore, the update of the degradation model is expected to affect the temporal dependencies of
125 retrieval accuracy. The retrieval results obtained using this model show that the temporal dependency of the XCO₂ bias against the TCCON measurement is reduced with respect to those using the current model in Someya and Yoshida (2020).



3.3 Solar irradiance spectra

The solar irradiance spectra used in the V02 algorithm were created using the baseline estimated from the report by Dr. R. Kurucz and the Fraunhofer lines personally provided by Dr. G. C. Toon (Yoshida et al., 2013). The baseline and Fraunhofer lines were updated in V03. The baseline was estimated using the Total and Spectral Solar Irradiance Sensor–1 Hybrid Solar Reference Spectrum (TSIS–1 HSRS; Coddington et al., 2021). Fraunhofer lines were obtained from version 2016 of Toon (2015b).

3.4 Gas absorption coefficient database

In the radiative transfer calculation of retrieval processing, gas absorption coefficients are obtained by interpolating look-up tables (LUTs) as the functions of temperature, pressure, and wavenumber. The LUTs are created using several databases, and the referenced databases were updated (Table 1.) Mendonca et al. (2017) found that the CH₄ retrieval using HITRAN2008 depends on the solar zenith angle. In the V02 retrievals, the residuals at several H₂O absorption lines increase with increasing water vapor because of the large uncertainties in spectroscopic parameters of H₂O. These problems can be resolved or mitigated by the updates. Associated with this update of LUTs, the scaling factor for O₂ absorption (see Section 2.3 of Yoshida et al., 2013 for details) is updated to 0.99556. Owing to the updates, the gas absorption coefficient database used in V03 retrievals is common to that used in the NIES SWIR L2 retrieval algorithm for TANSO–FTS–2 on GOSAT–2.

3.5 Other changes

In the NIES retrieval algorithm, the empirical noise model was estimated as the quadratic function of the signal-to-noise ratio to define the error covariance matrix (Yoshida et al., 2013). The coefficients of the functions in the V03 algorithm were updated due to the abovementioned changes. The empirical noise is not applied to the H₂O sub-band.

Post-screening is applied to the result after the retrievals, and one of the screening items is the spectral residual. The retrieval results with the mean squared of the residuals normalized with spectral noise larger than the thresholds are screened and not included in the L2 product. The thresholds were re-evaluated as 1.2, 1.2, 1.2, and 1.3 for the O₂ A, WCO₂, CH₄, and SCO₂ sub-bands, respectively. The threshold is undefined for the H₂O sub-band due to its large variability in water vapor concentrations.

Tables 2 and 3 summarize the retrieval setup for the V03 algorithm and the pre/post-screening procedures for the V02 and V03 algorithms.



4 Results

4.1 Spectral fitting accuracy

155 Figure 1 shows the spectral residuals at each sub-band obtained in April 2009 and April 2020 over land from V02.90. These are differences between the simulated radiance spectra using posterior states and the observed spectra. In each sub-band presented in the figure, the residuals exhibit some spectral dependencies. In the O₂ A sub-band, the residuals at the edges of the sub-band are larger than those in the central region and the structures of the O₂ absorption are seen. In the WCO₂ and CH₄ sub-bands, the residuals have relatively fine structures related to the gas absorptions, though those at the edges and in
160 the center are flattened. Figure 2 shows the spectral residuals same as Fig. 1, except that V03.00 is used. Compared with Fig. 1, the wavenumber dependencies of the residuals are decreased and the retrievals seem to be well fitted in Fig. 2. Same figures over the ocean are shown in Fig. 3 and 4. Same as over land, the fitting accuracies of V03.00 are found to be better than those of V02.90 in the O₂ A, WCO₂, and CH₄ sub-bands. However, in the SCO₂ sub-band, the residual has a significant spectral dependency, and it corresponds to the CO₂ absorption structure. The root mean squares of the averaged spectral
165 residuals in April 2020 shown in the figures are summarized in Table 4. The values from V03.00 are lower than the values from V02.90/91 and the spectral fitting accuracies are improved except for the SCO₂ sub-band over the ocean.

The abovementioned differences in spectral residuals between V02.90 and V03.00 are mainly owing to the update of solar irradiance and gas absorption cross-section database. This is because the treatment of clouds has a smaller impact on the fine structure of the residuals, and there are slight spectral dependencies of differences between the new and old degradation
170 models shortly after the launch. The update of solar irradiance decreased the relatively large wavenumber dependencies, such as the large residuals around 6,375 cm⁻¹ and the large wavenumber dependency around 6,000 cm⁻¹ shown in Fig. 3. Updating the gas absorption cross-section database significantly improves the fitting accuracy in the CH₄ sub-band and substantially decreases the fine structure of the residuals. The O₂ A sub-band is flattened, and the differences between the center and edges of the sub-band are decreased by both the updates of solar irradiance and gas absorption coefficients.
175 However, in the O₂ A sub-band, some differences between 2009 and 2020 remain. One possible reason of this is the degradation model. The number of components used to construct the degradation model in the O₂ A sub-band is smaller than the other band because the contributions of the primary components are large. The temporal differences are possibly due to the contributions by the other components which are not considered in the construction of the degradation model.

Figure 4 shows the significant spectral dependencies of the residuals obtained from V03.00 in the SCO₂ sub-band over the
180 ocean. In this figure, the baselines of the simulated radiance spectra seem to have some biases. Over the ocean, the surface state is described only by the surface wind speed in the retrieval and the spectral baseline is not adjusted (unlike that in over land). The spectral structure corresponding to CO₂ absorption is found in this figure. This can be result of changes in retrieved CO₂ to reduce residuals due to baseline bias. This can lead to a bias in the retrieved XCO₂.



4.2 Global distribution of the retrieval results

185 In this section, we show the difference in the retrieval results between V02.90/91 and V03.00. The data from the launch to 2021 are used for both the versions. Global distributions of the retrieved XCO₂, XCH₄, and the number of observations for V02.90/91, V03.00, and their differences are shown in Fig. 5. The XCO₂ from V03.00 over land is approximately the same as that from V02.90/91. Conversely, over the ocean, the XCO₂ from V03.00 is several ppm lower than that from V02.90/91. This difference arises due to the spectral residual in the SCO₂ sub-band mentioned in Section 4.1.

190 The XCH₄ from V03.00 is lower than that from V02.90/91 globally. It is largely decreased in the middle and low latitudinal areas. Although it is difficult to isolate the impacts of each update on the retrieval results, our sensitivity test revealed that the XCH₄ over land changed by approximately 7 ppb depending on whether solar irradiance spectra are updated or not. On the other hand, the other test with the replacement of the gas absorption table shows smaller changes in XCH₄ over land. These may indicate that the decrease in XCH₄ is mainly because of the update of the solar irradiance spectra.

195 The number of observations over land is increased significantly because the 2 μm cloud screening is not applied in V03 retrievals. Because the XCO₂ values over land from V02.90/91 and V03.00 have only slight differences, the addition of the cirrus cloud parameters is effective to increase the number of observations. However, the number of observations over the ocean is decreased, except in the intertropical convergence zone, where cirrus clouds frequently exist because the residuals in the SCO₂ sub-band are increased, and more observations are filtered through the post-screening process in the V03.00
200 retrieval. The numbers of observations from the V02.90/91 and V03.00 XCO₂ products are shown in Table 5. The V03.00 product increases the number of observations obtained over land and the mixed surface of land and ocean, by 12.7% and 22.3% compared with the V02.90/91 product, respectively. In opposite, it decreases by 20.3% over the ocean. Overall, the number of available observations from V03.00 is 2.3% larger than that from V02.90/91.

Figure 6 shows the global distributions of the ancillary parameters, the difference between the retrieved and a priori surface
205 pressures (Δ Ps), retrieved temperature shift, large-particle AOT, and the COT from V02.90/91 and V03.00. These results are obtained only from the observations that passed the post-screening process those with large AOT and COT (>0.1) are excluded. The general Δ Ps patterns are similar for V02.90/91 and V03.00. Over land, negative biases are slightly improved in V03.00. Over the ocean, positive biases are large in the high latitudes of the southern hemisphere for V02.90/91 and low latitudes for V03.00. The horizontal pattern of Δ Ps over land in the middle and low latitudes seems to correspond to that of
210 the difference in XCH₄ shown in Fig. 5. The relatively large decrease in XCH₄ in low latitudes over the ocean could be attributed to the changes in Δ Ps. Negative biases of temperature shift decreased globally for V03.00, and those over the ocean for V02.90/91 changed to slightly positive biases. Although the relatively large negative biases remain in inland China for V03.00, those in Europe and America for V02.90/91 become smaller for V03.00. The AOT of large particles at 1.6 μm decreased globally, especially over the ocean for V03.00. The COT is obtainable only for V03.00. Although the observations
215 with large COT values are rejected by post-screening, the relatively large values are seen in the tropical regions, where cirrus clouds are frequently present.



4.3 Comparison with TCCON measurements

The retrieved XCO₂ and XCH₄ are validated using the TCCON measurements in this section. The TCCON sites used in this study are listed in Table A1. The GOSAT measurements used for the comparisons are selected within $\pm 2^\circ$ from each TCCON site. The TCCON measurements within ± 30 min from the GOSAT measurement time are averaged for comparison. We used the data from the launch to 2021. Currently, the newest TCCON product, version GGG2020, is provided and we used this version in this analysis. However, not all sites have produced their full GGG2020 time series at the time of writing. The main changes between GGG2020 and the previous version, GGG2014, are found on the TCCON wiki page (<https://tcon-wiki.caltech.edu/Main/DataDescriptionGGG2020>). The data amount of GGG2020 is currently smaller than that of GGG2014 because of stricter quality control processes, but much of these data should be recovered in the near future. In particular, measurements collected before 2011 are sparse.

The comparison results for V03.00 and V02.90/91 versus TCCON are shown in Table 6. Bias means the average of the differences between GOSAT and TCCON, and the standard deviations are calculated from these differences. The GOSAT measurements are categorized according to the surface state and the gain (high: H or middle: M) setting of the FTS measurement. The observations containing both the land and ocean surfaces in the instantaneous field of views of TANSO-FTS are not used here. The number of observations with gain H from V03.00 is larger than that from V02.90/91 over land. On the other hand, those with gain M from V03.00 are slightly smaller than those from V02.90/91. The sites used for gain M are only two sites, Pasadena and JPL which are very close to each other and located near Los Angeles. Over the ocean, the number of observations from V03.00 decreases. There are no substantial changes in the standard deviations of the differences for XCO₂ and XCH₄ in all the situations, although the biases are different between V03.00 and V02.90/91 in some cases.

The biases and standard deviations of the XCO₂ from V03.00 are close to those from V02.90/91 over land. Considering these results, the XCO₂ from V03.00 has similar qualities as that from V02.90/91 over land. Meanwhile, the bias of the XCO₂ from V3.00 is larger and more negative than that from V02.90/91 over the ocean. This issue is consistent with the results presented in Section 4.2 and is because of the fitting accuracy shown in Section 4.1. Therefore, the bias correction seems necessary for the XCO₂ from V03.00 over the ocean.

As shown in Section 4.2, the XCH₄ from V03.00 decreased from those from V02.90/91. Over land, the absolute values of the XCH₄ from V03.00 are slightly larger with gain H and significantly smaller with gain M than those from V02.90/91. Over the ocean, the bias from V03.00 is larger, although a smaller data amount is available. Therefore, we need to investigate the biases over the ocean with a larger amount of data in the future.

The validation results over land with gain H in the stricter match-up condition of $\pm 0.1^\circ$ are shown in Table 7 to investigate these differences more precisely. Because of the spatial variability of GHGs, the validation with the stricter condition is more reliable, especially for XCH₄. Unfortunately, there are no match-up data found over land with gain M and over the ocean in this match-up condition. In this table, the absolute values of bias and standard deviation of the XCH₄ from V03.00 are



250 smaller than those from V02.90/91. Therefore, the quality of the XCH₄ from V03.00 can be regarded as almost the same as
or better than those from V02.90/91.

Inter-site and temporal variability of the differences between GOSAT and TCCON are investigated using the match-up
condition of $\pm 0.1^\circ$. The data with more than 10 match-up observations were used for both the investigations of inter-site and
temporal variability. 10 TCCON sites (Burgos, Caltech, JPL02, Lauder02, Lauder03, Lamont, Paris, Saga, Sodankyla, and
255 Tsukuba) were found as the match-up data sites for investigating inter-site variability. Site biases, average site bias, and site-
to-site variability were calculated as the mean differences from TCCON for individual sites, an average of site biases, and a
standard deviation of site biases, respectively. The average site biases and the site-to-site variabilities from V03.00 are -0.01
and 1.74 ppm for XCO₂ and -2.14 and 9.33 ppb for XCH₄, respectively. Those from V02.90/91 are -0.02 and 1.72 ppm for
XCO₂ and 5.99 and 9.12 ppb for XCH₄. The average site biases and the site-to-site variabilities of XCO₂ are similar for
260 V03.00 and V02.90/91. For XCH₄, although the site-to-site variability from V03.00 is slightly higher than that from
V02.90/91, the average site bias is smaller in V03.00. Temporal variability was calculated from the annual mean of the
differences between GOSAT and TCCON. The time series of the annual mean differences are shown in Fig. 7. Temporal
trends of the XCO₂ from V03.00 and V02.90/91 are similar after 2014 though the values from V02.90/91 are respectively
large in 2012 and 2013. Although the values from V03.00 are generally lower than those from V02.90/91, the same trends
265 are found for XCH₄. The standard deviations of the annual mean values from V03.00 and V02.90/91 are 0.42 and 0.52 ppm
for XCO₂ and 1.44 and 2.06 ppb for XCH₄ respectively. Thus, V03.00 exhibits smaller temporal variability than V02.90/91
in this analysis.

4.4 Evaluating the long-term trend using in situ measurements

The TCCON sites used in the previous section were mainly obtained over land. However, as noted in Section 2.2, there is an
270 issue with the decadal growth rate of XCO₂ estimated using the V02.90/91 product over the ocean. In this section, we
evaluate the long-term trends of XCO₂ using in situ measurement data.

NIES has observed CO₂ via air sampling on ships (Tohjima et al., 2005), and at ground stations (Nomura et al., 2017; 2021)
in southwestern Asia and the western Pacific Ocean for more than a decade. CO₂ in the upper troposphere has been observed
by aircraft in the CONTRAIL project (Machida et al., 2008). In addition, NOAA Global Monitoring Laboratory has
275 provided flask sampling and in situ measurement data on the western Pacific islands (Conway et al., 1994; Lan et al., 2022).
The data used in this study are listed in Table A2. The products from these in situ measurements are appropriate to evaluate
the GOSAT product in terms of the stability of data accuracy. Because these observations obtain the concentrations of the
trace gases at the surfaces or at certain atmospheric levels, that are not column-averaged, they are not directly comparable
with the XCO₂ obtained from GOSAT. Therefore, we only focus on the decadal increasing trend of CO₂ from both products
280 in this study. Further, we only evaluate the CO₂ trends because the comparison of CH₄ is more complicated due to its large
vertical gradient and variability. For aircraft measurement, only the data obtained at altitudes of 5 km or higher were used.
The 22 areas are defined using $12^\circ \times 12^\circ$ grid boxes and the CO₂ concentrations obtained from GOSAT and each in situ



measurement platform were monthly averaged in each area for comparison. The locations of the in situ measurements and areas used in this analysis are depicted in Fig. 8.

285 Figure 9 shows the time series of the differences between the XCO₂ from the GOSAT V02.90/91 or V03.00 product and CO₂ concentration from each in situ measurement platform. Over land, the growth rates of CO₂ estimated from the GOSAT V02.90/91 and V03.00 products are consistent with that from the in situ measurements within 1 ppm/decade. This value is close to the difference between TCCON and the in situ measurements. On the other hand, the growth rate for V02.90/01 over the ocean is 1.7 ppm/decade smaller than that from the in situ measurements. However, the difference in the growth rate for
290 V03.00 is improved to 0.0 ppm/decade although the biases are negatively large as shown in the previous sections.

The main cause of this trend of the GOSAT V02.90/91 product over the ocean is estimated as the sensitivity degradation of TANSO-FTS. Although the degradation is considered in the V02 algorithm with the degradation model according to Yoshida et al. (2012), the degradations after 2012 are the expected ones. The error of this degradation model generates a gap in the spectral baseline between the observed and simulated spectra. The difference in trend is not significant over land
295 because the gap can be adjusted by simultaneously retrieving surface albedo. In the NIES retrieval algorithm, only the wind speed is retrieved as a surface property over the ocean and not surface albedo. Therefore, the difference in the trend of CO₂ between GOSAT V02.90/91 and the in situ measurements could have resulted from the increasing error of the degradation model with time. This improvement of the trend of V03.00 over the ocean is mainly because of the update of the degradation model described in Section 3.2 as the other updates do not vary over time.

300 4.5 Bias correction

Because the V03.00 product has biases particularly for XCO₂ over the ocean, as shown in the previous sections, those should be corrected. We used TCCON GGG2014 for this bias correction because insignificant changes were found in XCO₂ between both versions and the available amount of data is larger than GGG2020. The site information of TCCON GGG2014 used in this study is listed in Table A3. The bias correction for XCH₄ is not processed here since those are largely changed
305 between GGG2014 and GGG2020. Since the GGG2020 is not fully available, we plan to correct XCH₄ based on GGG2020 after more stations are published. The bias correction strategy is the same as that used in the V02.95/96 products (NIES GOSAT project, 2020). The bias correction of the XCO₂ for V03 is a function of AOT, ΔPs, and surface albedo at the O₂A sub-band. Multiple linear regression analysis was used to estimate the coefficients. The TCCON data from 2009 to 2019 is used as the reference data. The changes in the XCO₂ from V03.00 after the correction are shown in Fig. 10. Only minor
310 differences are found over land. The negative bias over the ocean revealed in the previous sections is corrected by this procedure. The mean changes of the XCO₂ by the bias correction are +0.55 ppm over land and +6.31 ppm over the ocean. The bias-corrected version of the XCO₂ product plans to be released as V03.05.



5. Summary and conclusions

315 The retrieval algorithm for the GOSAT TANSO–FTS SWIR L2 product from NIES was updated to generate the next version, the V03 product. The main changes in the V03 algorithm compared with the current retrieval algorithm (V02) are as follows:

1. COT and CTP are retrieved simultaneously with the GHGs instead of the cirrus cloud screening using the $2\mu\text{m}$ band in the pre-screening processing
2. The degradation model of TANSO–FTS is updated to that of Someya and Yoshida (2020)
3. Solar irradiance spectra are updated to those produced from TSIS-1 HSRS and the version 2016 of Toon (2015b)
- 320 4. Gas absorption coefficient tables are updated using several new references

The retrieval results show that the spectral fitting accuracies are successfully improved, and the systematic spectral residuals in the V02.90/91 product are reduced in the O_2A , WCO_2 , and CH_4 sub-bands. Conversely, the residual in the SCO_2 sub-band increases over the ocean with a systematic spectral structure corresponding to the CO_2 absorptions. This increase in the residual is mainly attributed to a gap in the spectral baseline between observed and simulated spectra.

325 The amount of data from V03.00 is larger than that from V02.90/91 over land and the mixed surfaces mainly owing to the change in the treatment of clouds, although it is smaller over the ocean because of the residual in the SCO_2 sub-band. Overall, the amount of data from V03.00 increased by 2.3% compared with that from V02.90/91.

The direct comparison of V03.00 with V02.90/91 and the validation using TCCON measurements shows that the quality of XCO_2 from V03.00 is almost the same level as that from V02.90/91 over land—the update achieves an increase in the 330 available data without reducing the quality of the retrieved XCO_2 . On the other hand, the XCO_2 from V03.00 over the ocean is negatively biased and the bias correction is necessary. Although the bias XCH_4 over land with gain H from V03.00 is slightly larger than that from V02.90/91 in the match-up condition of $\pm 2^\circ$, it is smaller in the stricter condition, $\pm 0.1^\circ$. Regarding the spatial variability in CH_4 , the results obtained with the stricter match-up condition are more reliable, and V03.00 improves the quality of XCH_4 . The standard deviations of the XCH_4 differences between GOSAT and TCCON are 335 similar for V02.90/91 and V03.00. Considering these validation results and the improvement in fitting accuracies, the quality of the XCH_4 from V03.00 is comparable to or better than that from V02.90/91. In addition, the investigation of site-to-site and temporal variability of XCO_2 and XCH_4 biases from V03.00 demonstrates that their site-to-site variabilities are the approximately same level as, and the temporal variabilities are slightly smaller than those from V02.90/91.

340 The long-term trends of XCO_2 from both product versions are evaluated via in situ measurements. The V03.00 product resolves the issue that the decadal CO_2 growth rate estimated from the V02.90/91 products over the ocean is 1.7 ppm/decade lower than that from the in situ measurements.

345 Although the V03 retrieval algorithm has an issue to be resolved for XCO_2 over the ocean, the objectives of the update, increase in data, and improvement of the fitting accuracy are generally achieved over land. Notably, the increase in data of 13% over land and the improvements of the temporal variabilities of biases are helpful for the flux inversions or emission estimates of CO_2 and CH_4 . NIES plans to release the L2 V03.00 product and the bias-corrected V03.05 in near future.



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350 Author contributions

YS performed the investigation of the retrieval results, contributed to the development of the retrieval system, and prepared the manuscript. YY designed and developed the retrieval system, contributed to the investigation of the retrieval results, and edited the manuscript. HO and IM contributed to the development of the retrieval system and provided the TCCON data. SN, AK, and HM contributed to the investigation of the retrieval results. TM acquired funding. JL, VV, BH, YT, MS, RK, MZ,
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Conflicts of interest

The authors have no conflicts of interest, financial or otherwise, related to this study.



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Table 1: Summary of the optical parameter updates

Gas absorption	Reference database	
	V02	V03
O ₂	Tran et al. (2006) Tran and Hartmann (2008)	ABSCO V5.0 (Drouin et al., 2017)
CO ₂	Lamouroux et al. (2010)	
CH ₄	HITRAN 2008 (Rothman et al., 2009)	Devi et al. (2015; 2016) for the 2ν ₃ band of ¹² CH ₄ HITRAN 2016 (Gordon et al., 2017) for the others
H ₂ O	HITRAN 2008	ATM line list 2014 (Toon, 2015a)
H ₂ O continuum	MT_CKD V2.5.2 (Mlawer et al., 2012)	MT_CKD V3.2

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Table 2: Retrieval setup for the V03 product. COT and CTP are additional parameters from V02.

State vector	No. of elements	a priori	Uncertainty
CO ₂ mixing ratio	15	NIES-TM	estimated from NIES-TM
CH ₄ mixing ratio	15	NIES-TM	estimated from NIES-TM
H ₂ O mixing ratio	15	GPV (GSM)	estimated from GPV (GSM)
AOT (small particle)	6	SPRINTARS	0.5
AOT (large particle)	6	SPRINTARS	0.5
COT	1	0.1	0.05
CTP	1	150 hPa	30 hPa
Surface pressure	1	GPV (GSM)	5 hPa
Temperature shift	1	0 K	5 K
Surface albedo (over land)	2, 9, 11, 2, 2 (O ₂ A, WCO ₂ , CH ₄ , H ₂ O, SCO ₂ sub-band)	estimated from measured spectra	1
Wind speed (over ocean)	1	GPV (GSM)	estimated from GPV (GSM)
Zero level offset	1 (O ₂ A sub-band only)	0 W/cm ² /sr/cm ⁻¹	10 ⁻⁸ W/cm ² /sr/cm ⁻¹
Wavenumber dispersion factor	4 (O ₂ A, WCO ₂ , CH ₄ , SCO ₂ sub-band)	0	10 ⁻⁵



640 **Table 3: Summary of the pre/post-screening procedures for the V02 and V03 algorithm. The observation is rejected if more than one item satisfies the criteria.**

Item		Rejection criteria	
		V02	V03
Pre-screening	L1B quality	Bad	
	Out-of-band spectrum	Outlier	
	CAI cloud flag	Cloudy	
	CAI coherent (ocean)	Cloudy	
	2 μm band cloud flag	Cloudy	–
	Solar zenith angle	$> 70^\circ$	
	SNR	< 70 for O ₂ A sub-band	
	Land fraction	0 % $<$ and < 60 %	
Post-screening	No. of iteration	20	
	Mean squared residuals (O ₂ A, WCO ₂ , CH ₄ , and SCO ₂ sub-bands)	$> 1.2, 1.2, 1.3, \text{ and } 1.4$	$> 1.2, 1.2, 1.2, \text{ and } 1.3$
	Degree of freedom for signal	< 1	
	AOT (1.6 μm)	> 0.1	
	Blended albedo	> 1	
	Surface wind speed	$< 0.1 \text{ m/s}$ or $> 20 \text{ m/s}$	
	Absolute difference between retrieved and a priori P _s	$> 20 \text{ hPa}$	
	retrieved COT	–	> 0.1

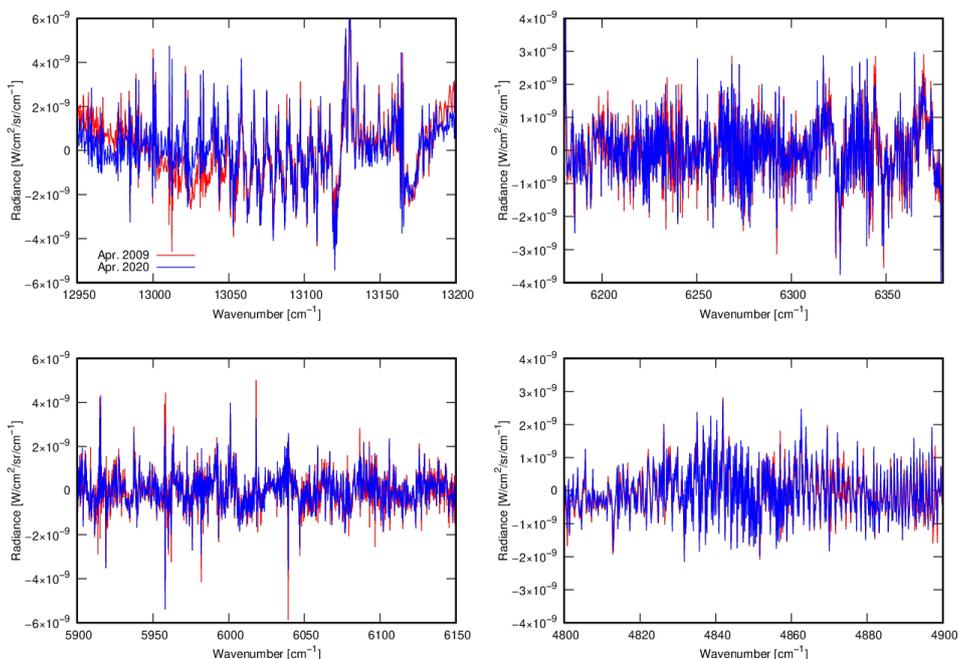


Fig. 1: Averaged spectral residuals (simulated minus observed) at $\text{O}_2 \text{ A}$ (top-left), WCO_2 (top-right), CH_4 (bottom-left), and SCO_2 (bottom-right) sub-bands in April 2009 (red) and April 2020 (blue) over land obtained from V02.90.

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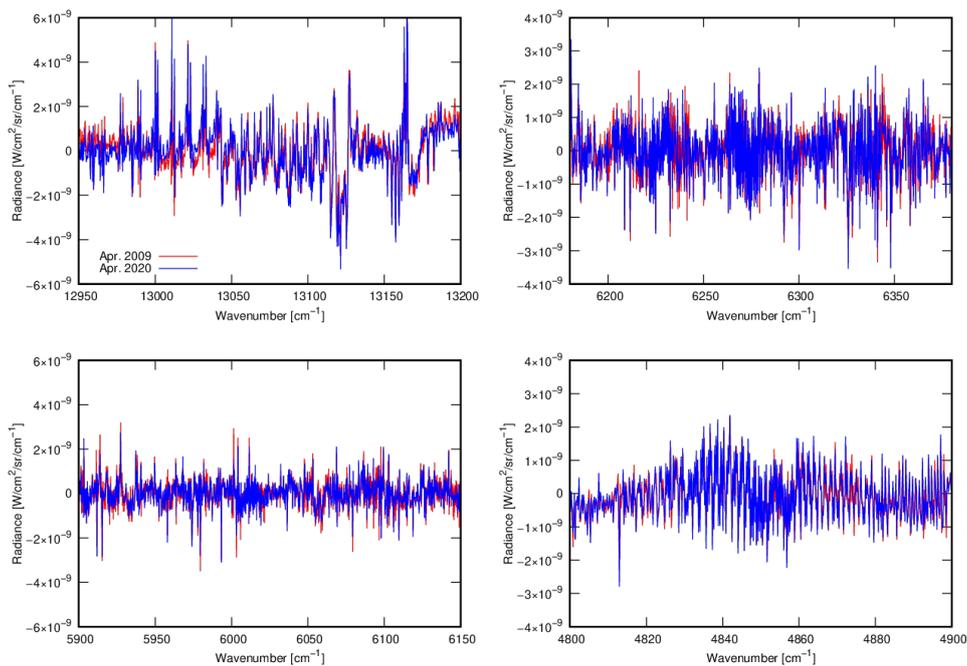


Fig. 2: Same as Fig. 1 but for V03.00.

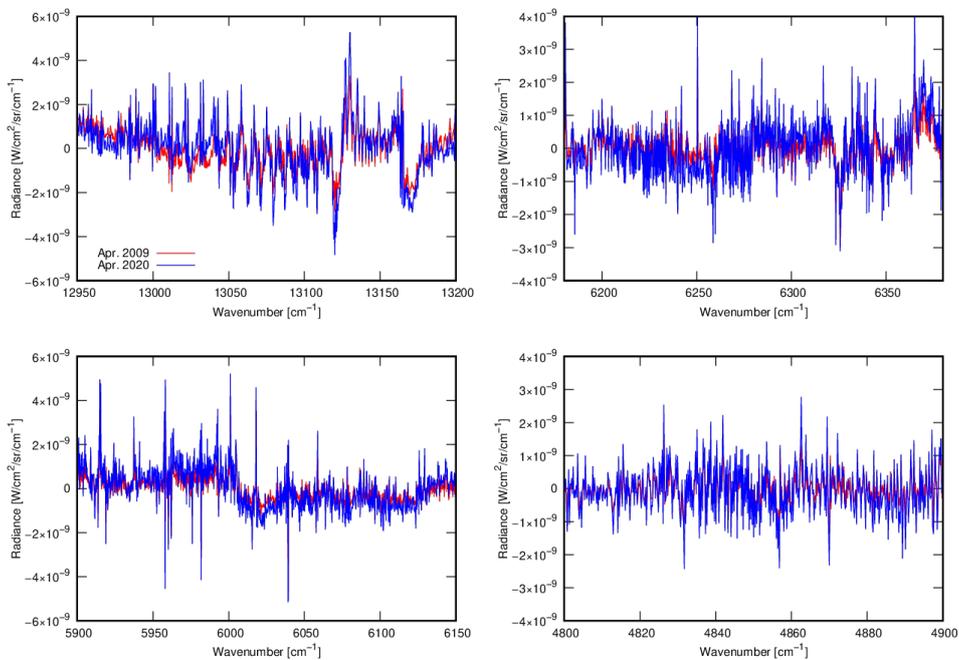


Fig. 3: Same as Fig. 1 but for over the ocean.

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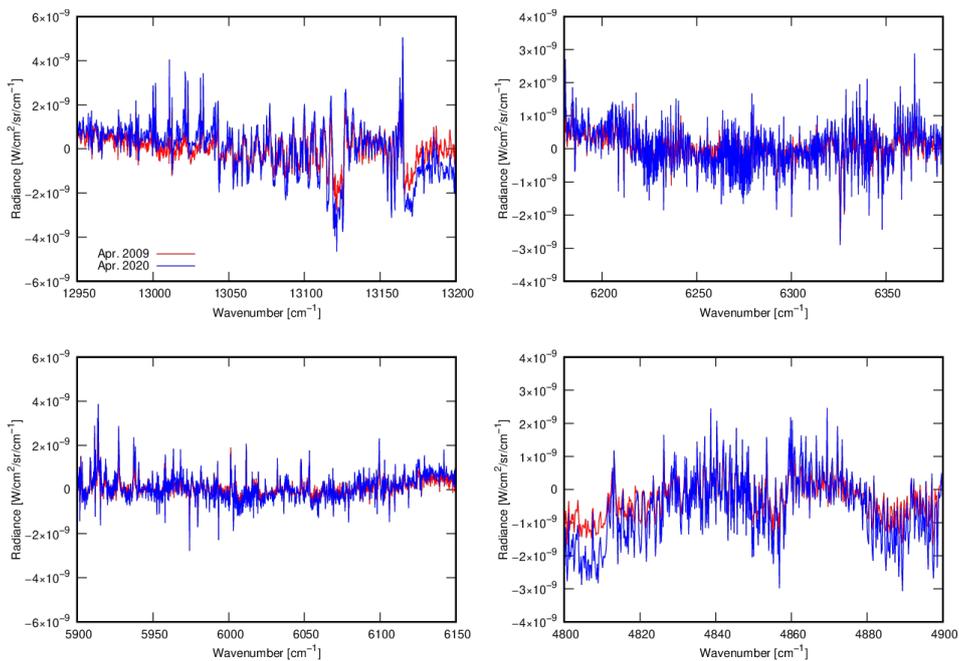
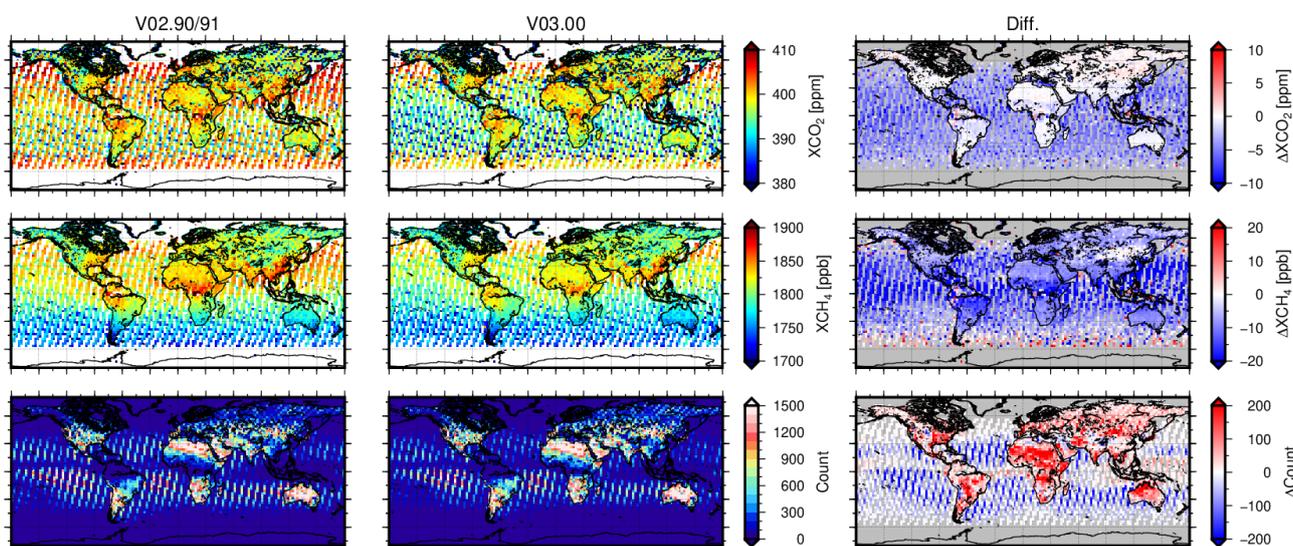


Fig. 4: Same as Fig. 3 but for V03.00.



655 **Table 4: Root mean squares of the averaged spectral residuals for each sub-band in April 2020. The unit is $\times 10^{-9} \text{ W/cm}^2/\text{sr/cm}^{-1}$.**

		O ₂ A	WCO ₂	CH ₄	SCO ₂
V02.90/91	Land	1.429	0.973	0.811	0.834
	Ocean	1.219	0.859	0.980	0.762
V03.00	Land	1.217	0.854	0.612	0.799
	Ocean	1.161	0.687	0.613	1.206



660 **Fig. 5: Global distributions of XCO₂ (top), XCH₄ (middle), and the number of observations (bottom) for V02.90/91 (left), V03.00 (middle), and their differences (right) from the launch to 2021.**

Table 5: Number of observations from the V02.90/91 and V03.00 XCO₂ products and their differences for each surface type from the launch to 2021.

	V02.90/91	V03.00	Difference (%)
Land	960,394	1,082,768	+12.7%
Ocean	557,488	444,477	-20.3%
Mixed	130,836	159,960	+22.3%
Total	1,648,718	1,687,205	+2.3%

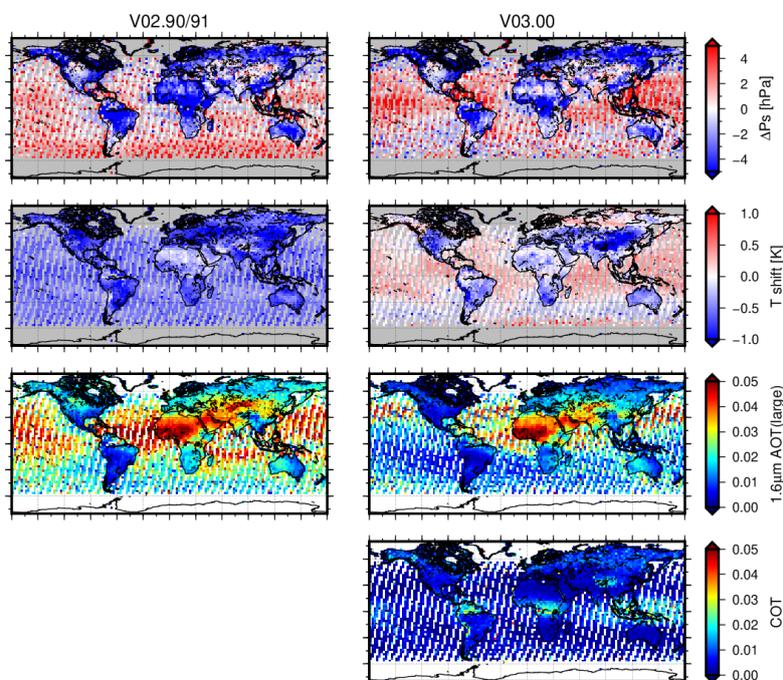


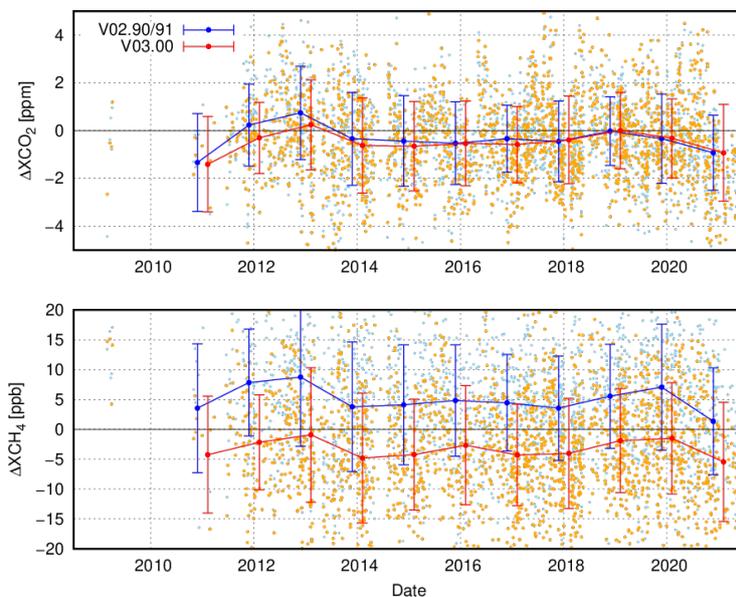
Fig. 6: Distributions of the averaged ΔP_s , T shift, large particle AOT at $1.6 \mu\text{m}$, and COT at $0.55 \mu\text{m}$ from V02.90/91 and V03.00. COT is obtainable only from V03.

670 Table 6: Validation results of V03.00 and V02.90/91 against the TCCON measurements version GGG2020 with the match-up condition of $\pm 2^\circ$. The mean values of the differences between TCCON and GOSAT (Bias) and their standard deviations (SD) are shown for each combination of surface conditions and gain settings.

Version	Surface/Gain	CO ₂			CH ₄		
		No. of data	Bias (ppm)	SD (ppm)	No. of data	Bias (ppb)	SD (ppb)
V02.90/91	Land/H	7357	-0.56	2.13	7365	2.97	11.94
	Land/M	1385	-0.79	1.89	1385	8.13	19.17
	Ocean/H	72	-1.63	2.62	72	5.60	15.43
V03.00	Land/H	8780	-0.61	2.20	8790	-4.23	11.97
	Land/M	1360	-0.88	1.97	1360	-0.19	19.29
	Ocean/H	61	-8.12	2.81	61	-9.71	14.60

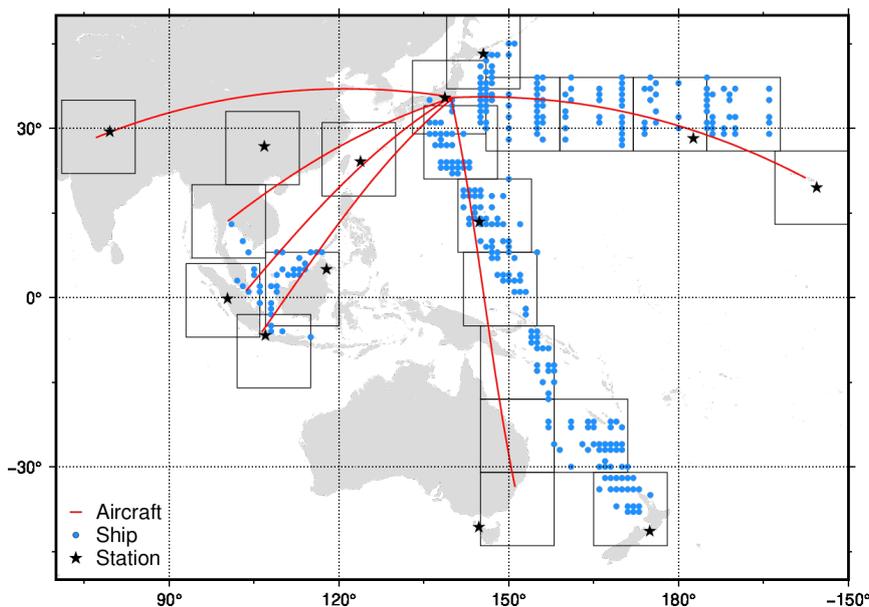
675 Table 7: Validation results of V03.00 and V02.90/91 over land with gain H against the TCCON measurement version GGG2020 in the match-up condition of $\pm 0.1^\circ$.

Version	CO ₂			CH ₄		
	No. of data	Bias (ppm)	SD (ppm)	No. of data	Bias (ppb)	SD (ppb)
V02.90/91	1743	-0.31	1.76	1744	4.81	9.81
V03.00	2111	-0.43	1.81	2112	-3.30	9.68



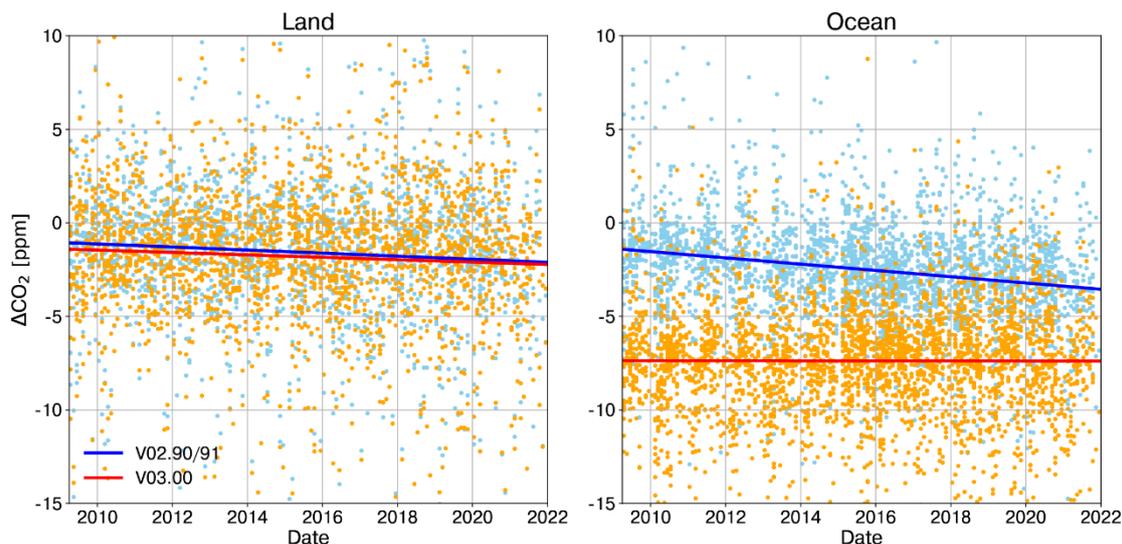
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Fig. 7: Annual mean differences of the GOSAT L2 product and TCCON GGG2020 in the match-up condition of $\pm 0.1^\circ$ for XCO_2 (top) and XCH_4 (bottom). The red and blue lines indicate V03.00 and V02.90/91, respectively. The annual mean plots are slightly shifted between V02 and V03 for visibility. Each individual observation from V03.00 and V02.90/91 is plotted as orange and light-blue dots.

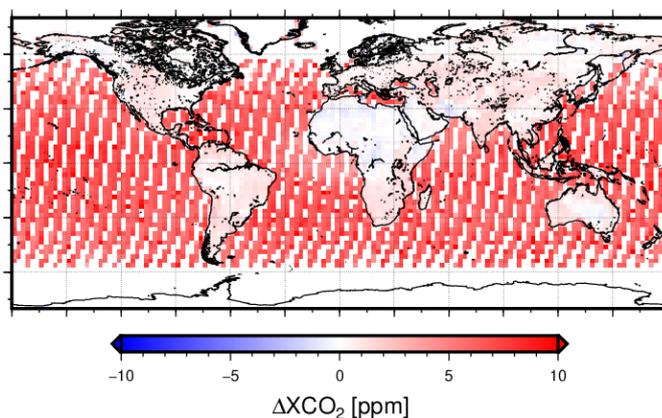


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Fig. 8: Main route or locations of the aircraft (red line), ship (blue dot), and station (black star) measurements. The areas for comparison with the GOSAT data are shown in boxes. Here, we only show the main routes of the aircraft measurements (Haneda/Narita to Delhi, Bangkok, Singapore, Jakarta, Sydney, and Honolulu) accounting for more than 97% although the remaining data contain the other routes (Haneda/Narita to Taipei, Kuala Lumpur, Denpasar, Cairns, Brisbane, and Guam).



690 **Fig. 9:** Time series of the differences between GOSAT and in situ measurements (GOSAT minus in situ measurements) over land (left) and the ocean (right). The differences in monthly averaged values for V02.90/91 (light blue) and V03.00 (orange) in each area are plotted. The regression lines are plotted as the blue and red lines.



695 **Fig. 10:** Difference of XCO₂ between V03.00 and the bias-corrected one (bias-corrected minus V03.00) averaged from the launch to 2021 within a 2.5°×2.5° grid.



Table A1: Site information of the TCCON GGG2020 data used for validation

Site	Latitude	Longitude	Start date	End date	Reference
Bremen	53.10N	8.85E	1/6/2009	6/24/2021	Notholt et al. (2022)
Burgos	18.533N	120.650E	3/3/2007	4/30/2020	Morino et al. (2022a)
Caltech (Pasadena)	34.136N	118.127W	9/20/2012	3/1/2022	Wennberg et al. (2022a)
East Trout Lake	54.354N	104.987W	10/3/2016	3/6/2022	Wunch et al. (2022)
Four Corners	36.707N	108.48W	3/16/2013	10/3/2013	Dubey et al. (2022a)
Indianapolis	39.861N	86.004W	8/23/2012	12/1/2012	Iraci et al. (2022)
JPL02	34.202N	118.175W	5/19/2011	5/14/2018	Wennberg et al. (2022b)
Karlsruhe	49.100N	8.439E	1/15/2014	12/22/2021	Hase et al. (2022)
Lauder01	45.038S	169.684E	6/28/2004	2/19/2010	Sherlock et al. (2022a)
Lauder02	45.038S	169.684E	1/2/2013	9/30/2018	Sherlock et al. (2022b)
Lauder03	45.038S	169.684E	10/2/2018	3/30/2021	Pollard et al. (2022)
Lamont	36.604N	97.486W	7/6/2008	2/27/2022	Wennberg et al. (2022c)
Manaus	3.213S	60.598W	9/30/2014	7/27/2015	Dubey et al. (2022b)
Nicosia	35.141N	33.381E	9/3/2019	6/1/2021	Petri et al. (2022)
Orleans	47.97N	2.113E	8/29/2009	3/8/2021	Warneke et al. (2022)
Paris	48.846N	2.356E	9/23/2014	6/16/2021	Té et al. (2022)
Park Falls	45.945N	90.273W	5/26/2004	2/28/2022	Wennberg et al. (2022d)
Reunion	20.901S	55.485E	3/1/2015	7/18/2020	De Mazière et al. (2022)
Rikubetsu	43.457N	143.766E	6/24/2014	6/30/2021	Morino et al. (2022b)
Saga	33.241N	130.288E	7/28/2011	6/30/2021	Shiomi et al. (2022)
Sodankyla	67.367N	26.631E	3/5/2018	10/18/2021	Kivi et al. (2022)
Tsukuba	36.051N	140.122E	3/28/2014	6/28/2021	Morino et al. (2022c)
Xianghe	39.75N	116.96E	6/14/2018	11/30/2021	Zhou et al. (2022)



Table A2: In situ measurement data availability

Platform/site	Citation
Aircraft	Atmospheric CO ₂ mole fraction data of CONTRAIL-CME, DOI: 10.17595/20180208.001
Ship	https://soop.jp (partially on request)
NIES station	
Ochi-ishi	Continuous Observational Data of Atmospheric CO ₂ Mixing Ratios at Cape Ochi-ishi, DOI: 10.17595/20160901.002
Mt. Fuji	Daily Observational Data of Atmospheric CO ₂ Mixing Ratios at the Summit of Mt. Fuji, DOI: 10.17595/20170616.001
Nainital	Atmospheric Carbon Dioxide Dry Air Mole Fraction at Nainital, India, DOI: 10.17595/20220301.001
Hateruma	Continuous Observational Data of Atmospheric CO ₂ Mixing Ratios on Hateruma Island, DOI: 10.17595/20160901.001
Guiyang	On request
Danum Valley	On request
Bukit Kototabang	On request
Serpong	On request
Bogor	On request
Cibeureum	On request
NOAA flask/in-situ	Atmospheric Carbon Dioxide Dry Air Mole Fractions from the NOAA GML Carbon Cycle Cooperative Global Air Sampling Network, 1968-2021, Version: 2022-07-28, DOI: 10.15138/wkgj-f215
Midway	Atmospheric Carbon Dioxide Dry Air Mole Fractions at Sand Island, Midway, https://gml.noaa.gov/aftp/data/trace_gases/co2/flask/surface/txt/co2_mid_surface-flask_1_ccgg_month.txt
Guam	Atmospheric Carbon Dioxide Dry Air Mole Fractions at Mariana Islands, Guam, https://gml.noaa.gov/aftp/data/trace_gases/co2/flask/surface/txt/co2_gmi_surface-flask_1_ccgg_month.txt
Cape Grim	Atmospheric Carbon Dioxide Dry Air Mole Fractions at Cape Grim, Tasmania, https://gml.noaa.gov/aftp/data/trace_gases/co2/flask/surface/txt/co2_cgo_surface-flask_1_ccgg_month.txt
Baring Head	Atmospheric Carbon Dioxide Dry Air Mole Fractions at Baring Head, New Zealand, https://gml.noaa.gov/aftp/data/trace_gases/co2/flask/surface/txt/co2_bhd_surface-flask_1_ccgg_month.txt



Table A3: Site information of the TCCON GGG2014 data used for bias correction.

Site	Latitude	Longitude	Start date	End date	Reference
Ascension	7.916S	14.333W	5/22/2012	10/31/2018	Feist et al. (2014)
Anmeyondo	36.538N	126.331E	2/2/2015	4/18/2018	Goo et al. (2014)
Bialystok	53.23N	23.025E	3/1/2009	10/1/2018	Deutscher et al. (2015)
Bremen	53.10N	8.85E	1/22/2010	2/24/2021	Notholt et al. (2014)
Burgos	18.533N	120.650E	3/3/2017	3/31/2020	Morino et al. (2018a)
Caltech (Pasadena)	34.136N	118.127W	9/20/2012	12/29/2020	Wennberg et al. (2015)
Darwin	12.425S	130.892E	8/28/2005	4/30/2020	Griffith et al. (2014a)
East Trout Lake	54.354N	104.987W	10/7/2016	9/6/2020	Wunch et al. (2017)
Edwards	34.958N	117.882W	7/20/2013	12/31/2020	Iraci et al. (2016a)
Eureka	80.05N	86.42W	7/24/2010	7/6/2020	Strong et al. (2017)
Four Corners	36.707N	108.480W	3/16/2013	10/4/2013	Dubey et al. (2014a)
Garmisch	47.476N	11.063E	7/16/2007	4/1/2021	Sussmann and Rettinger (2015)
Hefei	31.91N	117.17E	9/18/2015	10/23/2018	Liu et al. (2018)
Indianapolis	39.861N	86.004W	8/23/2012	12/1/2012	Iraci et al. (2016b)
JPL02	34.202N	118.175W	5/19/2011	5/14/2018	Wennberg et al. (2016a)
Karlsruhe	49.100N	8.439E	4/19/2010	12/22/2021	Hase et al. (2015)
Lauder01	45.038S	169.684E	6/29/2004	12/9/2010	Sherlock et al. (2014a)
Lauder02	45.038S	169.684E	2/2/2010	10/31/2018	Sherlock et al. (2014b)
Lauder03	45.038S	169.684E	10/3/2018	12/31/2020	Pollard et al. (2019)
Lamont	36.604N	97.486W	7/6/2008	12/28/2020	Wennberg et al. (2016b)
Manaus	3.213S	60.598W	10/1/2014	6/24/2015	Dubey et al. (2014b)
Nicosia	35.141N	33.381E	8/31/2019	3/9/2021	Petri et al. (2022)
Orleans	47.97N	2.113E	8/29/2009	3/8/2021	Warneke et al. (2014)
Paris	48.846N	2.356E	9/23/2014	6/22/2020	Té et al. (2014)
Park Falls	45.945N	90.273W	6/2/2004	12/29/2020	Wennberg et al. (2017)
Reunion	20.901S	55.485E	9/16/2011	7/18/2020	De Mazière et al. (2014)
Rikubetsu	43.457N	143.766E	11/16/2013	9/30/2019	Morino et al. (2016)
Saga	33.241N	130.288E	7/28/2011	12/29/2020	Kawakami et al. (2014)
Sodankyla	67.367N	26.631E	5/16/2009	10/20/2020	Kivi et al. (2017)



Tsukuba	36.051N	140.122E	8/4/2011	9/30/2019	Morino et al. (2018b)
Wollongong	34.406S	150.879E	6/26/2008	6/30/2020	Griffith et al. (2014b)
Zugspitze	47.42N	10.98E	4/24/2015	4/1/2021	Sussmann and Rettinger, (2018)

705