



Retrieval of greenhouse gases from GOSAT and greenhouse gases and carbon monoxide from GOSAT-2 using the FOCAL algorithm

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Abstract.

Recently, the Fast atmospheric trace gas retrieval (FOCAL) algorithm has been applied to measurements of the Greenhouse gases Observing SATellite (GOSAT) and its successor GOSAT-2. FOCAL has been originally developed for Orbiting



Carbon Observatory-2 (OCO-2) retrievals with the focus on the derivation of carbon dioxide (XCO_2). However, depending on
5 the available spectral windows, FOCAL also successfully retrieves total column amounts for other atmospheric species. Here,
we show new results from updated GOSAT and GOSAT-2 FOCAL retrievals. The main focus is placed on methane (XCH_4 ;
full physics and proxy product), water vapour (XH_2O) and the relative ratio of semi-heavy water (HDO) to water vapour
(δD). Due to the extended spectral range of GOSAT-2 it is also possible to derive information on carbon monoxide (XCO) and
nitrous oxide (XN_2O) for which we also show first results. We also present an update on XCO_2 from both instruments.

10 Compared to the previous product version (v1), the number of valid XCO_2 data could be significantly increased in the
updated version (v3.0) by 50% for GOSAT and about a factor of two for GOSAT-2. All FOCAL data products show reasonable
spatial distribution and temporal variations. Comparisons with TCCON (Total Carbon Column Observing Network) result in
station-to-station biases which are generally in line with the reported TCCON uncertainties.

With this updated version of the GOSAT-2 FOCAL data, we provide a first total column average XN_2O product. Global
15 XN_2O maps show a gradient from the tropics to higher latitudes in the order of 15 ppb, which can be explained by variations
in tropopause height. The new GOSAT-2 XN_2O product compares well with TCCON. Its station-to-station variability is lower
than 2 ppb, which is about the magnitude of the typical N_2O variations close to the surface. However, both GOSAT-2 and
TCCON measurements show that the seasonal variations in the total column average XN_2O are in the order of 8 ppb peak-to-
peak, which can be easily resolved by the GOSAT-2 FOCAL data.

20 1 Introduction

Global, long-term data sets of atmospheric constituents are essential to improve our understanding of the behavior of the Earth's
atmosphere. Remote sensing by satellite instruments provides a way to derive large scale information from measurements. In
a time of changing climate, reliable remote sensing data products gain importance, as they are a crucial input, e.g. for models
used for climate projections and air quality simulations. Information about the global distribution of greenhouse gases and
25 about their sources and sinks plays an important role in this context.

Several retrieval methods exist for the derivation of atmospheric information from satellite measurements. In many cases
these approaches are based on spectral information from different wavelength regions, and they concentrate on, and are opti-
mised for, a single product. However, the derivation of a specific product usually requires the consideration of various additional
atmospheric constituents and processes.

30 Recently, Noël et al. (2021) presented a first version (v1.0) of a XCO_2 data product from GOSAT (Greenhouse gases
Observing SATellite; Kuze et al., 2009, 2016) and GOSAT-2 (Suto et al., 2021) measurements in the near-infrared (NIR)
and shortwave infrared (SWIR) spectral regions derived with the FOCAL (Fast atmOspheric traCe gAs retrievalL) method
(Reuter et al., 2017a, b). FOCAL is based on a full-physics retrieval in which scattering is approximated by a single layer. The
Noël et al. (2021) paper focused on the XCO_2 results, but the application of FOCAL to the GOSAT instruments includes the
35 determination of various other atmospheric quantities. In the current paper, we present results from an updated version (v3.0) of
the GOSAT and GOSAT-2 FOCAL retrieval. Although we will also show the results for the new XCO_2 data, the main focus of



the paper is on the presentation and initial validation of the additional quantities that can be derived with a single retrieval, thus showing the capabilities of the FOCAL method beyond XCO_2 . In the following, in addition to XCO_2 , we present the GOSAT and GOSAT-2 FOCAL results for methane (XCH_4 ; full physics and proxy product), water vapour (XH_2O) and semi-heavy water (HDO, respectively its ratio to H_2O denoted as δD). For GOSAT-2, we will also show results for carbon monoxide (XCO) and first nitrous oxide (XN_2O) data.

For some of the gases derived from GOSAT measurements, several data products exist. The Japanese National Institute for Environmental Studies (NIES) provides operational XCO_2 , XCH_4 (Yoshida et al., 2013) and XH_2O products (Dupuy et al., 2016). NASA also released a XCO_2 product based on the ACOS retrieval, recently described by Taylor et al. (2022). A precursor of the FOCAL XCO_2 product v1.0 from Noël et al. (2021) is the BESD v01.04 product, also from the Institute of Environmental Physics (IUP) Bremen (Heymann et al., 2015). This is a near-real-time product produced for the Copernicus Atmospheric Monitoring Service (CAMS, <https://atmosphere.copernicus.eu/> (last access: 30-July-2020)). It is planned to replace this with a near-real-time version of the FOCAL XCO_2 product described in this paper in the near future. Several GOSAT products are produced for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>; last access: 30-July-2020). In this context, the Netherlands Institute for Space Research (SRON) provides XCO_2 and XCH_4 data (Butz et al., 2011; Schepers et al., 2012). Similar products are also generated by the University of Leicester (Cogan et al., 2012; Parker et al., 2011, 2020). The ratio of HDO to H_2O (δD) was derived by Frankenberg et al. (2013) and Boesch et al. (2013).

For GOSAT-2, operational XCO_2 , XCH_4 , XCO and XH_2O SWIR products have been released by NIES (see <https://prdt.gosat-2.nies.go.jp/>, last visited 6 June 2021). There is no XN_2O product for GOSAT-2 available yet.

The main aim of the current study is to give an overview of the large number of newly available FOCAL data products for GOSAT and GOSAT-2. To get an impression about the quality of these products, we compare them with ground-based measurements from the Total Carbon Column Observing Network (TCCON; Wunch et al., 2011). For GOSAT we also include comparisons with other available XCO_2 and XCH_4 GOSAT data sets.

The paper is structured as follows: After this introduction, we present the input data used in this study in section 2. We then describe the updated retrieval algorithm in section 3, followed by the results of the study (including first validation) in section 4. Finally, we summarise everything in the conclusions (section 5). Additional information is given in the appendix.

2 Input Data

The input data used in this study are essentially the same as for the v1.0 product described in Noël et al. (2021) with some updates described in the following.

As input spectra, we use calibrated GOSAT and GOSAT-2 L1B radiances of the three NIR/SWIR bands at around 0.76, 1.6 and 2.0 μm . All data until the end of 2020 are processed. For GOSAT, we use product version V220.220, extended by V230.230 for about the last two months of 2020. The GOSAT-2 L1B product version is now V102.102. The instrumental line shape (ILS) data are the same as in Noël et al. (2021).



The solar irradiance and solar induced fluorescence (SIF) reference spectra are unchanged. The cross sections have been updated; we now use data from HITRAN2016 (Gordon et al., 2017, downloaded on 23 March 2021) in combination with updated cross sections from the NASA (National Aeronautics and Space Administration) ACOS/OCO-2 project, i.e. ABSCO v5.1 data (Benner et al., 2016; Devi et al., 2016).

As in Noël et al. (2021), surface properties are obtained from the Global Multi-resolution Terrain Elevation Data (GMTED2010; Danielson and Gesch, 2011) of the U.S. Geological Survey (USGS) and the National Geospatial-Intelligence Agency (NGA). Meteorology is taken from ECMWF (European Centre for Medium-range Weather Forecasts) ERA5 model data (Hersbach et al., 2020).

There has been a change in the a priori profile data used for XCO₂ and XCH₄. These are now derived using a Simple cLimatological Model for atmospheric CO₂ and CH₄, respectively, called SLIMCO2 and SLIMCH4 (see Appendix A for details). All other a priori data and the related uncertainties are unchanged compared to v1.0. The SLIMCO2 and SLIMCH4 data are also used in the bias correction for XCO₂ and XCH₄. As “truth”, we use a subset of the SLIM data from 2019 that has been selected based on a comparison with TCCON data (see Noël et al., 2021, for a detailed description).

We still use the same TCCON data version GGG2014 for comparison, but now for the extended time period until the end of 2020. All involved TCCON stations and related references are listed in Table 1.

In addition to the validation with ground-based data we also include comparisons with other GOSAT data sets for XCO₂ and XCH₄, namely the ACOS v9r XCO₂ product from NASA (Taylor et al., 2022); the full physics and proxy products from the University of Leicester (UoL XCO₂ and XCH₄ FP v7.3, UoL XCH₄ proxy v9.0; Cogan et al., 2012); the full physics and proxy products from SRON (RemoTeC FP XCO₂ and XCH₄ v2.3.8, RemoTeC XCH₄ proxy product v2.3.9; Butz et al., 2011); and the operational bias-corrected GOSAT XCO₂ and XCH₄ products from NIES v02.9x (Yoshida et al., 2013).

3 Retrieval Algorithm

The retrieval used in this study is a three-step approach consisting of pre-processing, processing and post-processing. Since the retrieval method is essentially the same as the one described in Noël et al. (2021) for product version 1.0 we will describe in the following only the differences applied for the updated product version (v3.0; v2 was an unreleased internal version). Most relevant changes for the current product version were in the pre- and post-processing parts.

3.1 Pre-Processing

The pre-processing collects and prepares all data required for the processing. This step especially includes the measured GOSAT and GOSAT-2 spectra, and geolocation and matching meteorological and topographic information (from ECMWF ERA5 and GMTED2010). Furthermore, some initial filtering (especially for clouds) is performed. For the new FOCAL products, some filter limits of the pre-processing have been relaxed to increase final the data yield: We now use a maximum solar zenith angle of 90° and also latitudes up to ±90°. In v1.0, both limits were set to 70°. Note that these limits are applied for pre-processing; further filtering is done later during post-processing, depending on the different products (see section 3.3). All



other filtering (including the cloud filter) is unchanged compared to v1.0. The main difference in pre-processing to v1.0 is, therefore, that for v3.0 high latitudes are not necessarily filtered out before processing. Furthermore, as mentioned above, we now use SLIMCO₂ and SLIMCH₄ data as a priori for XCO₂ and XCH₄.

3.2 Processing

105 The processing for v3.0 is very similar to the one of v1.0. It is based on the Fast atmOspheric traCe gAs retrievalL (FOCAL) algorithm described in Reuter et al. (2017b). We now use a modified version of FOCAL, which assumes isotropic instead of Lambertian scattering at the scattering layer. The fitting windows are the same as in v1.0, but we also fit H₂O in the NIR band (see Tab. 2).

The state vector elements (see Tab. 3) are also almost the same as in v1.0; however, we increased the degrees of the back-
110 ground polynomials to improve the fit residuals such that now all fitted polynomials are of degree 3 except for the small solar induced fluorescence (SIF) windows where we use a degree of 1 and the XN₂O window where a degree of 4 is used.

All quantities in the state vector are retrieved simultaneously. For CO₂, CH₄ and H₂O we derive profiles on 5 layers which are then converted to total column averages. δD, XCO and XN₂O are derived via scaling factors. The XCH₄ proxy product is derived after the retrieval from these full physics products (see below). In the case of GOSAT-2, all scattering parameters as
115 well as methane, water vapour and δD are only fitted in windows 1 to 6 (i.e. those spectral ranges which are also available for GOSAT). This is done for consistency reasons.

As in v1.0, before the retrieval for GOSAT – but not GOSAT-2 – we compute a spectral correction factor to account for changes in the spectral calibration with time. This factor is now obtained from the spectral difference of Fraunhofer lines in the solar irradiance and measured radiance in the SIF window, which is more stable than the least-squares fitting procedure used
120 in v1.0. This new method only corrects for shifts on the scale of one spectral sampling interval (0.2 cm⁻¹); this, however, is sufficient, as additional spectral shift and squeeze factors are determined in the later retrieval.

We also use a noise model to correct the uncertainties of the GOSAT and GOSAT-2 spectra estimated during pre-processing and consider possible forward model uncertainties in the retrieval. This noise model is the same as in v1.0, but we re-computed the parameters for all fitting windows based on an input data set consisting of one day per month in 2019 for both GOSAT and
125 GOSAT-2. The resulting parameters are, however, similar for v1.0 and v3.0.

3.3 Post-Processing

The main changes between v1.0 and v3.0 occur in the post-processing. The overall concept of our new approach is that we tried to establish a generic, mostly automated procedure that provides reproducible results and thus can be applied to all gases under consideration. However, it still allows for an optimisation for each product.

130 The following post-processing steps are in general applied to all products:

1. Basic filtering.
2. Quality filtering.



3. Bias correction (for CO₂ and CH₄ only).

Note that, in contrast to v1.0, there is no longer a filter on the derived bias applied after the bias correction.

135 The XCH₄ proxy product is computed during post-processing from:

$$XCH_4^{\text{proxy}} = XCH_4^{\text{retrieved}} \frac{XCO_2^{\text{apriori}}}{XCO_2^{\text{retrieved}}} \quad (1)$$

This means we normalise the retrieved full physics XCH₄ by the retrieved full physics XCO₂ (both without bias correction) and use as reference the a priori XCO₂. Note that this is different to e.g. the SRON XCH₄ proxy product (Wu et al., 2021), which is derived from a dedicated non-scattering retrieval using a different wavelength region (6045 – 6138 cm⁻¹). The uncertainty
140 of the proxy product is then determined via error propagation. The XCH₄ proxy product is then treated in post-processing as the other products.

3.3.1 Basic filtering

In contrast to v1.0, the basic filtering does not involve filtering based on scientific knowledge, e.g. by using pre-described limits of scattering parameters or product uncertainties. This is no longer done as these fixed limits removed too many possibly valid
145 data points, especially in the case of GOSAT-2.

Therefore, the basic filtering now only includes the filtering for good convergence (χ^2 smaller than 2) and a maximum residual-to-signal ratio (RSR) as a function of the noise-to-signal ratio (NSR). This is done in the same way as for v1.0 (see Noël et al., 2021), but with the updated noise model parameters mentioned above. This part of the basic filtering is common for all products.

150 For GOSAT, the RSR filters for all fitting windows (1–6) are applied to all data products. In case of GOSAT-2, for consistency reasons we also apply only the RSR filters for windows 1–6 to those products, that are also available from GOSAT (i.e. XCO₂, methane and water vapour products). For the others, i.e. XCO and XN₂O, we only apply RSR filters from the NIR (windows 1 and 2, where most of the scattering information comes from) and those windows where these gases are retrieved, namely window 8 for XCO and window 7 for XN₂O. This is to avoid that e.g. a valid XCO₂ measurement is filtered out due to a bad
155 XN₂O fit (or vice versa).

In addition to this, we apply a filter on a maximum solar zenith angle (SZA) of 75°, because we cannot expect good data products for too low lighting conditions. This SZA filter is applied for all products except for water vapour, because requirements on water vapour are not as strict as e.g. for XCO₂. This is why we do not apply this strict filter already in pre-processing (where we only limit the SZA to 90°, see above).

160 3.3.2 Quality filtering

The quality filtering is product-specific, but follows the same strategy for each target gas. In general, we perform independent filtering for water and land surfaces.

The filtering out of low-quality data was done in v1.0 by a random forest filter. However, as explained in Noël et al. (2021), the performance of this filter method was limited as it essentially filtered out fewer data than expected. Therefore, we replaced



165 this filtering for v3.0 with a filter procedure that has already been successfully used in OCO-2 retrievals; details can be found in Reuter et al. (2017a). This procedure is based on a minimisation of the local variance. This is done by computing, for a subset of the data, the variance of the difference between the retrieved quantity and its median on a $15^\circ \times 15^\circ$ grid.

Based on this subset, we check which variables from a given list of the candidate variables perform best in reducing the local variance when removing data corresponding to the highest or lowest 1% of each variable. This action defines a new upper or
170 lower limit for this variable. We repeat this until a prescribed amount of data is removed. The output of this procedure is a list of “best” variables and their new filter limits.

This subset has been generated from data of 2019 for GOSAT and GOSAT-2, to which the basic quality filter as described above has been applied. Note that – in contrast to v1.0 – this subset no longer depends on the reference database used in the bias correction.

175 A general problem with this filtering method is that it tends to filter out values from regions with higher noise, which might result in reduced coverage at higher latitudes if too many data are to be filtered out.

Therefore, we apply this filtering in two steps: First, using the variance filter method, we only determine limits for (only) the scattering optical depth parameters derived in the retrieval for a given percentage of data to be filtered out (P_τ).

After applying this filter, we further reduce the number of data by another percentage (P_V) by using the variance filter method
180 again, but now for an extended list of possible filter candidates. This list of variables has been largely reduced compared to v1.0. It now only comprises results from the retrieval, namely the uncertainties (but not values) of the retrieved target species, χ^2 , scattering parameters and their uncertainties, the polynomial coefficients and their uncertainties, wavelength shift/squeeze and their uncertainties, and surface roughness. We explicitly no longer include geolocation / viewing geometry parameters and surface elevation to avoid that data are filtered out due to e.g. a specific geographical region. The retrieved CO₂ gradient
185 at the surface is also not used anymore, as this might result in filtering out scenes with too high CO₂ in the boundary layer close to a point source. However, because of the large number of fitting windows this still leaves a list of about 200 possible parameters. To reduce this to a reasonable number, we run this variance filter twice: first, with the full list, then with only the best 10 parameters. This number of 10 parameters is only an upper limit, which has been chosen by checking that adding more parameters does not further reduce the variance significantly. Depending on the relevance of individual quantities even fewer
190 parameters are needed in some cases.

The choice of the number of data to be filtered out is – as always – a trade-off between the remaining number of data points and data quality. For the v3.0 data, we determined suitable numbers for P_τ and P_V by looking at the resulting data quality (maps and validation) for different settings. As for the SZA filter, the optical depth filter is not applied for each product. We use the same values for GOSAT and GOSAT-2; these are listed in Tab. 4. The finally selected filter variables and their limits
195 are specific for each product, surface and instrument. They are given in the Appendix in Tab. A1 to A12.

3.3.3 Bias correction

After filtering out data as described above, we apply a bias correction to XCO₂ and the XCH₄ full physics and proxy products. The overall procedure is the same as described in detail in Noël et al. (2021). The bias correction is based on a random



forest regression using, as for v1.0, the ten most relevant parameters and a random forest database as input. These have been
200 determined as described in Noël et al. (2021), using as input the variance-filtered test subset of data as mentioned above
and a reference database giving the “true” XCO₂ and XCH₄. This reference database has been generated from a subset of
daily SLIMCO₂ and SLIMCH₄ data (see Appendix A) for 2019, which agree within ±0.5 ppm for XCO₂ and ±10 ppb for
XCH₄ with corresponding TCCON data. The “best” parameters have been chosen from essentially the same list of candidate
205 variables used in the variance filter, but now extended with surface elevation and type, solar zenith angle, viewing zenith angle,
continuum signal and flags for quality and instrument gain.

The final choice of bias correction parameters and their relevance is shown in Fig. A7 for GOSAT and Fig. A8 for GOSAT-2
(see Appendix B).

We also perform a correction of the retrieved XCO₂ and XCH₄ uncertainties via a linear function. The coefficients of this
function (see Tab. 5) are determined in a similar way as described in Noël et al. (2021), but instead of TCCON data we now
210 use data from the SLIMCO₂/SLIMCH₄ reference database as “true” values.

4 Results

All GOSAT and GOSAT-2 data until the end of 2020 have been processed. Fig. 1 shows the final number of valid FOCAL data
as a function of time for the different products. The numbers are different for each product because of the individual filtering
(see above). For comparison, the numbers for the v1.0 XCO₂ products are also shown. Fig. 1a compares the number of yearly
215 GOSAT-FOCAL XCO₂ data with other available GOSAT data products from SRON, the University of Leicester (UoL), NIES
and NASA (ACOS product). A similar comparison is shown in Fig. 1b for XCH₄ full physics and proxy products. The resulting
amount of data for the GOSAT-FOCAL water vapour products is shown in Fig. 1c. The yield of valid FOCAL products was
improved in v3.0 compared to v1.0. The number of valid FOCAL XCO₂ and methane results exceeds those of all other GOSAT
data sets.

220 The total number of GOSAT-2 FOCAL products (see Fig. 1d) was also improved, but is still lower than for GOSAT. This
is because a larger fraction of data are already removed during the basic filtering due to larger residuals / less convergence.
This hints at possible issues with the radiometric calibration or an incomplete instrument model used by FOCAL, neglecting
important instrument features, e.g. currently unconsidered effects of remaining polarisation sensitivities of the instrument.

4.1 Global maps

225 For each of the different data products an example map comprising a mean for April 2019, gridded to 5° × 5°, is shown in
Fig. 2 for GOSAT and in Fig. 3 for GOSAT-2. In all maps, grid points that were only based on a single measurement have
been omitted to avoid outliers. The spatial patterns of methane, water vapour, δD and XCO₂ look very similar for GOSAT and
GOSAT-2. GOSAT-2 data show in general fewer gaps over the oceans, but with smaller latitudinal coverage. The latter is due
to the currently applied RSR filtering for GOSAT-2, which especially removes data over water surfaces. Note that over the year
230 the spatial range of valid data varies according to illumination conditions.



The XCO₂ data show higher values in the northern than in the southern hemisphere as expected during spring time.

For methane, the known source regions in the US, Africa and Asia are clearly visible, as well as the inter-hemispheric gradient. The spatial coverage of the proxy product is much larger than for the full physics product, especially at higher latitudes.

235 Water vapour (XH₂O) also shows the expected behaviour: large values in the tropics and lower values at higher latitudes. All δD values are in the expected range (about 0 to -300‰); they also decrease from the tropics to higher northern and southern latitudes. This is because water vapour generated in the tropics by strong evaporation is transported to higher latitudes, during which the heavier HDO decreases more rapidly via precipitation than H₂O. The observed spatial distribution of δD is in line with the maps shown in Frankenberg et al. (2013).

240 For GOSAT-2 there are also data for carbon monoxide (XCO) and XN₂O. In the XCO map the expected source regions in China, Indonesia and Africa (fossil fuel combustion, biomass burning) are apparent over the otherwise quite smooth and constant background. The transport of XCO from the equatorial African fire regions to the west over the Atlantic ocean due to the trade winds is clearly visible.

The XN₂O product shows an overall decrease of the background XN₂O from the tropics to higher latitudes in the order of
245 15 ppb. Such gradients were also observed by the IASI (Infrared Atmospheric Sounding Interferometer) instrument on Metop (Barret et al., 2021), however, we see larger differences. This could be related to the sampling of the XN₂O data. Furthermore, the IASI data shown in Barret et al. (2021) refer to the mid-troposphere over the ocean only, whereas the GOSAT-2 FOCAL data are total column averages over all surfaces. The latitudinal XN₂O gradient can, in principle, be explained by the variation of the tropopause height. As most of the XN₂O is contained (and well mixed) in the troposphere, the total column average is
250 larger in the tropics (where the tropopause is high) than at higher latitudes. We also see increased XN₂O over central Africa. This is also visible in IASI data and probably related to convection (see Ricaud et al., 2009).

4.2 Time series

Time series of all GOSAT-FOCAL data products for different latitudinal regions are depicted in Fig. 4. These plots show the expected temporal behaviour: A seasonal cycle is visible in all data sets; amplitudes and/or phase differ for northern and
255 southern latitudes with usually more variability in the north.

The methane full physics and proxy products show a similar temporal variation with increasing XCH₄ (about 10 ppb per year, in line with recent annual changes from NOAA ground-based measurements, see https://gml.noaa.gov/ccgg/trends_ch4/ (last access 11 January 2022)). Small differences between the average XCH₄ full physics and the proxy products can be explained by the broader spatial coverage of the proxy product.

260 For water vapour (XH₂O), the seasonal cycles in the northern and southern hemispheres are shifted by about six months, in line with the seasonal shift of the intertropical convergence zone (ITCZ). On the global scale, these seasonal variations largely average out. No clear trend is visible in the GOSAT water vapour data from 2009 to 2020.

Average values of δD vary between about -180‰ and -120‰. As for water vapour, seasonal variations are small in the global average, but year-to-year variations in the seasonal cycle are larger for δD.



265 The GOSAT-2 time series (see Fig. 5) show similar temporal variations to the GOSAT data, but of course, they only cover the years 2019 and 2020. XCO shows similar values and seasonal variations for all latitudinal regions except for the southern hemisphere, where XCO is on average about 30 ppb lower than in the northern hemisphere, probably because most sources are around the equator or in the northern hemisphere extra-tropics.

The GOSAT-2 XN₂O also shows some seasonal variations of up to about 8 ppb peak-to-peak. However, this seasonality is at least partly a sampling effect. The background XN₂O, as shown in Fig. 3g, comprises larger values in the tropics than at higher latitudes. Because of the varying latitudinal coverage of GOSAT-2 ocean data throughout the year, the regions outside the tropics are not covered during all seasons, which introduces an apparent variation in the averages. This effect in principle applies to all data, but is especially pronounced for XN₂O, for which other spatial variations are low. In the tropics, the XN₂O data are always high, and the variations are much smaller. In fact, we see a slight increase in XN₂O of about 1 ppb per year, 275 which is about what is expected from ground-based measurements (see growth rate plots on the NOAA Global Monitoring Laboratory website; <https://gml.noaa.gov/hats/combined/N2O.html>, last access 30 June 2021). This result is also in line with IASI data (Barret et al., 2021).

4.3 TCCON comparisons

To assess the quality of the data, for each GOSAT and GOSAT-2 FOCAL product we perform a comparison with TCCON data 280 using the same procedure as in Noël et al. (2021); see also Reuter et al. (2019, 2020) for details.

For most gases, we also use the same collocation criteria: a maximum time difference of 2 h, a maximum spatial distance of 500 km and a maximum surface elevation difference of 250 m between satellite and ground-based measurement. However, for water vapour and carbon monoxide these limits are reduced to 1 h time difference and 150 km spatial distance to account for their higher variability. We only include stations with a minimum of 50 data points.

285 For XCO₂ and XCH₄ we also perform comparisons with other available GOSAT products from SRON, the University of Leicester, NASA(ACOS) and NIES.

From the comparisons, we derive the following main quantities:

- The mean station bias, defined as the mean of all biases at each station; this can be interpreted as a global offset to all stations.
- 290 – The station-to-station bias, defined as the standard deviation of the individual station biases. This can be interpreted as regional bias.
- The mean scatter, defined as the square root of the mean of the variances at each station. This is a measure for the single sounding precision.
- The seasonal bias, defined as the standard deviation (rms) of the seasonal variation of the difference FOCAL–TCCON 295 at each station. This is equivalent to a temporal bias.



Figs. 6 to 10 show the resulting bias and scatter for each GOSAT and GOSAT-2 product and TCCON station. Example time series for the TCCON station Lamont (US) are shown in Figs. 11 and 12. This station was selected because it provides good temporal coverage of TCCON data also for the GOSAT-2 time frame (2019–2020). All results of the comparisons are summarised in Tab. 6.

300 The mean station bias is mainly given for reference, because it is usually not relevant for applications that are only interested in the spatial and temporal gradients of the gas (like for XCO₂). The quantities station-to-station bias, seasonal bias, and mean scatter are more important as they describe the quality of regional and/or temporal gradients, which are, e.g., needed to quantify potential sources and sinks. The seasonal bias is derived from a trend model fit; therefore the corresponding values for GOSAT-2 are less reliable, because the time interval is only about two years. The number of stations and data points used in
305 the comparison depends on the different products, the collocation criteria and the length of the time series. Therefore, there are many fewer collocations for GOSAT-2. The XCH₄ proxy products, as well as the XH₂O and XCO products, have the largest number of collocations because of the relaxed filtering.

4.3.1 XCO₂ results

For GOSAT FOCAL v3.0 the XCO₂ station-to station bias is 0.51 ppm and the mean scatter 2.19 ppm. While the bias is
310 slightly reduced, the scatter is slightly larger than the values for v1.0 (0.56 ppm, 1.89 ppm, see Noël et al., 2021). This higher scatter is still acceptable noting the increased number of data points, which always increases the scatter, and an estimated 1- σ TCCON uncertainty of 0.4 ppm for XCO₂, see Wunch et al. (2010). Note that this relation between number of data and data points is due to the filtering, which is based on reducing the local variance by removing data points (see above). As stronger filtering therefore results in less data with a lower scatter.

315 The FOCAL values are also in quite good agreement with those from the other data sets, but still do not reach the low bias and scatter of the NASA ACOS product (0.44 ppm and 1.66 ppm).

The GOSAT-2 XCO₂ comparison results for v1.0 were considered less reliable because of the shortness of the time series (less than one year). For v3.0, we now have almost two years of data and, due to the updated product version, also a higher data yield, which results in almost 10 times more collocations with TCCON than in v1.0. We now get a station-to station bias of
320 0.91 ppm, which is still slightly higher compared to GOSAT but lower than in v1.0 (1.14 ppm). For GOSAT-2, the biases are typically negative for southern stations and positive for northern stations. The derived mean scatter of 2.02 ppm is somewhat lower than the v3.0 GOSAT value and slightly higher than the v1.0 scatter for GOSAT-2 (1.89 ppm). As mentioned above, this is related to the different number of data points.

The derived seasonal bias is low (0.33 ppm for GOSAT, 0.62 ppm for GOSAT-2). The seasonal variations of the TCCON
325 data at Lamont are well reproduced by the GOSAT and GOSAT-2 FOCAL data with no apparent offset, but the satellite data show a larger scatter (see Figs. 11a and 12a).



4.3.2 XCH₄ results

The full physics XCH₄ product for GOSAT has a station-to-station bias of 4.3 ppb, which is similar to the estimated 1- σ TCCON uncertainty from Wunch et al. (2010) of 3.5 ppb and also compares well to the other data products. The value for the
330 GOSAT FOCAL proxy product is 6.1 ppb, which is about 1–2 ppb higher than all other products but still in an acceptable range as it is better than the Copernicus systematic error threshold requirement of 10 ppb and close to the breakthrough requirement of better than 5 ppb (see Table 3 in Buchwitz et al., 2021). For GOSAT-2, we get a station-to-station bias of 4.7 ppb for the full physics XCH₄ product and 6.2 ppb for the proxy.

The mean scatter of the GOSAT and GOSAT-2 FOCAL XCH₄ product is around 12 ppb, which is slightly lower than for
335 the other data products. The seasonal bias for all GOSAT and GOSAT-2 products is around 3 ppb. For both instruments, the temporal variations of the FOCAL full physics and proxy XCH₄ products agree well with the Lamont TCCON data (see Figs. 11b,c and 12b,c). In general, the FOCAL data are systematically lower by a few ppb, in line with the observed mean station bias of around -3–6 ppb, see Tab. 6.

4.3.3 XH₂O results

340 Since water vapour is highly variable, the comparison results depend strongly on the involved TCCON stations. Because of the less strict filter criteria for XH₂O there are typically more data (and collocations) at higher latitudes than for the other full physics products. We get a similar mean scatter of about 300 ppm for GOSAT and GOSAT-2 FOCAL XH₂O. The station-to-station bias is 116 ppm for GOSAT and 152 ppm for GOSAT-2, which is even lower than the TCCON uncertainty of 200 ppm estimated by Wunch et al. (2010). The seasonal bias for GOSAT-2 is 110 ppm; for GOSAT it is even smaller (66 ppm). The
345 derived station-to-station biases and mean scatter values are in line with results derived for the OCO-2 FOCAL product (206 ppm and 293 ppm, respectively, see Reuter et al., 2017a). As also mentioned there, these high values can at least partly be attributed to the large natural variability of water vapour. This variability can also be seen in the time series at Lamont (Figs. 11d and 12d), which show the same seasonal variations of around 4000 ppm peak-to-peak for all data sets.

4.3.4 δ D results

350 For δ D we get station-to station biases of only 8.6‰ for both instruments; the mean scatter is about 32‰ for GOSAT and GOSAT-2. The seasonal bias for GOSAT is 6‰, the GOSAT-2 value is 13‰. The mean station bias is quite large (around -83‰ for GOSAT and GOSAT-2). This is slightly larger than corresponding values between about -20‰ and -70‰ derived from a GOSAT–TCCON comparison performed by Boesch et al. (2013) for data between April 2009 and June 2011. Note that there is no uncertainty estimate available for the TCCON δ D data, so all numbers given here should be treated with caution.
355 The Lamont time series (Figs. 11e and 12e) show a systematic offset between TCCON on GOSAT/GOSAT-2 in line with the mean station bias, but the seasonality is well reproduced, although the satellite data show a larger scatter.



4.3.5 XCO results

XCO and XN₂O products are only available for GOSAT-2, which covers a larger spectral range. The TCCON comparison for XCO reveals a station-to-station bias of 4.3 ppb, a mean scatter of 7.7 ppb and a seasonal bias of 2.8 ppb. In fact, the XCO bias and scatter varies strongly between the different TCCON stations (see Fig. 10a), but the derived values agree quite well with the TCCON uncertainty for carbon monoxide of 2 ppb. The data at Lamont (Fig. 12f) show that the temporal variation of XCO is well captured by the FOCAL product, but there is a systematic offset in line with the mean station bias of about 15 ppb.

4.3.6 XN₂O results

The FOCAL XN₂O is a new data product that is so far not available from other GOSAT-2 retrievals. For XN₂O we get from the TCCON comparison a station-to-station bias of 1.6 ppb and a mean scatter of 4.0 ppb. The seasonal bias is 1.6 ppb. Since the corresponding 1- σ TCCON uncertainty from Wunch et al. (2010) is 1.5 ppb we consider this as a reasonable agreement. The values for XN₂O are similar to the expected local XN₂O variability of a few ppb (see e.g. García et al., 2018), but it should be considered that the total column average has a larger variability due to e.g. variations in tropopause height than surface data. This can be seen from Fig. 12g: Both TCCON and GOSAT-2 observe total column seasonal variations with peak-to-peak differences of about 8 ppb, in line with the time series results. There is no visible bias between TCCON and GOSAT-2, but the scatter of the GOSAT-2 data is larger.

5 Conclusions

An updated version (v3.0) of the FOCAL retrieval algorithm has been applied to GOSAT and GOSAT-2 measurements in the NIR and SWIR spectral regions. This results in a variety of trace gas products, all derived within one retrieval. For both GOSAT instruments we determine full physics products for methane, water vapour and δD as well as a proxy methane product in addition to XCO₂. For GOSAT-2, also carbon monoxide and a nitrous oxide product are retrieved.

Overall, the yield of valid data could be improved in GOSAT and GOSAT-2 FOCAL v3.0. The number of XCO₂ full physics data has increased by about 50% for GOSAT and has even doubled for GOSAT-2. This is mainly due to relaxations in the filtering of data and improved post-processing. The proxy methane, carbon monoxide and XH₂O products even have about two times more data than the full physics products.

The spatial distribution of all gases and their temporal variation looks reasonable. For the new GOSAT-2 XN₂O we observe a gradient between the tropics and higher latitudes of about 15 ppb which can be explained by variations in the tropopause height. A similar gradient has been seen in IASI data.

The new GOSAT and GOSAT-2 products have been compared with ground-based TCCON data to get a first quality assessment. All FOCAL data agree with TCCON within the uncertainties of both data sets.



The accuracy of the GOSAT-2 FOCAL XN_2O is in the order of a few ppb for a single sounding. We expect this to be improved by averaging of data, such that e.g. monthly or annually gridded products can provide interesting information about XN_2O , especially since there are not many global satellite measurements available for this species.

390 *Data availability.* The GOSAT and GOSAT-2 FOCAL v3.0 data sets are available on request from the authors.

Appendix A: SLIMCO₂ and SLIMCH₄

The “Simple cLImatological Model for atmospheric CO₂ or CH₄” SLIMCO₂ or SLIMCH₄ has been developed to provide estimates of dry-air mole fraction profiles and column averages of atmospheric CO₂ or CH₄ with reasonable accuracy at minimum computational costs. A key application of SLIMCO₂ or SLIMCH₄ is to compute CO₂ or CH₄ a priori information
395 for remote sensing algorithms which is why it provides also estimates of the corresponding error covariance matrix which can be used, e.g., by optimal estimation frameworks.

The climatology database of SLIMCO₂ v2021 has been derived from 16 years (2003-2018) of CO₂ mole fraction data of NOAA’s CarbonTracker model version CT2019B Jacobson et al. (2020). It has the same $3^\circ \times 2^\circ$ spatial resolution as the used global CarbonTracker model fields. Temporally, it covers one year sampled in 36 time steps, corresponding to a grid
400 resolution of about 10 days. The climatology database of SLIMCH₄ v2021 has been derived from 13 years (2000-2012) of TM5-4DVAR CH₄ mole fraction data (Bergamaschi et al., 2013) with a spatial resolution of $6^\circ \times 4^\circ$. Temporally, it is sampled in 36 time steps, just as the climatology database of SLIMCO₂ v2021. Both databases feature a height grid with 20 layers. The height gridding is done in a way that each layer consists of the same number of dry-air particles so that the column-average can simply be computed by averaging the mole-fraction profile. When reading the climatology database, SLIM allows either
405 nearest neighbour or trilinear interpolation in longitude, latitude, and say of year. Additionally, SLIM is able to convert the height gridding to the one that is used, e.g., for the FOCAL OCO-2 XCO₂ retrieval using five height layers for CO₂.

First, we computed the global mean XGAS (XCO₂ or XCH₄) from the corresponding model for each January 1st (00:00 UTC) in the covered time period. In the next step, we went through all model time steps of the analysed period and subtracted the global mean XGAS, assuming linear growth within the years. Finally, we created the climatology databases by incremen-
410 tally computing the average and standard deviation of the gases mole-fraction of all growth corrected model time steps falling into the 10-days temporal grid-cells of the database. In this way, the created databases basically consist of growth-removed seasonal cycle anomalies.

In addition to the created 4D data fields, the database contains a table of annual growth rates obtained from NOAA (<https://gml.noaa.gov/ccgg/trends/gr.html>, last access 03.07.2021). Currently, the implemented table covers the time periods 1959-
415 2020 for CO₂ and 1984-2020 for CH₄, but it can be extended if needed to improve the quality of SLIM estimates in years before or after these periods. Fig. A1 shows the NOAA annual mean growth rates for CO₂ and CH₄ computed from global



marine surface data as stored in the database. As visible in the figure, the NOAA growth rate agrees well with the growth computed from the model data as described above.

In the following, we describe, how SLIM uses its database to estimate the CO₂ or CH₄ atmospheric dry-air mole fraction for a given longitude, latitude, and time. The database has been generated as follows: First, SLIM computes an estimate of the global average mole fraction by linear interpolation in the accumulated growth rates database. Note that extrapolation to dates outside of the spanned period is done by assuming a 10-years average growth rate (dashed lines in Fig. A1). This global average is added to the mole fraction anomaly interpolated from the corresponding 4D database field for the given longitude, latitude, and day of year.

Figures A2 shows examples of a global XCO₂ and XCH₄ map as read from the models (panels c and d) and in panels a and b the corresponding maps of SLIM XGAS values. Since the SLIM layers are defined such that the all contain the same number of dry air particles, the SLIM XGAS values can be computed as mean of all layer values. As one can also see in the difference maps (panels e and f), the large scale patterns such as north/south gradient are well reproduced and differences are mainly due the specific synoptic situation in the model field, which usually change from year to year and which, therefore, cannot be reproduced by a simple climatology. At the example of CO₂, the largest natural surface fluxes occur during the northern hemispheric growing season. Therefore, the largest deviations between CT2019B and SLIMCO₂ occur in the northern hemisphere in Fig. A2e.

By comparing one million randomly selected profiles in the period 2003-2018, we computed that the SLIMCO₂ XCO₂ is on average 0.1 ppm lower than the corresponding CarbonTracker values. The standard deviation of the difference amounts 0.57 ppm and the correlation coefficient between both quantities is 0.998 (see Fig. A3a). The corresponding experiment for SLIMCH₄ results in a mean difference of 3 ppb, a standard deviation of the difference of 7.2 ppb, and a correlation coefficient of 0.989 (see Fig. A3b).

The error covariance matrix for the 5-layered SLIMCO₂ profiles shown in Fig. A4a shows the largest uncertainties in the lowermost layer (approx. 1000-800 hPa) which is strongest influenced by the surface fluxes and the smallest uncertainties in the uppermost layer (approx. 200–0 hPa) including the stratosphere. The largest error correlations exist between the layers 1–4, whilst the uncertainties of layer 5 are relatively independent (Fig. A4b). For CH₄, the correlation structure is similar (Fig. A4d), but the largest uncertainties are observed in the stratosphere (Fig. A4c).

Also the comparison of SLIM with corresponding TCCON XGAS measurements show good overall agreement (Figs. A5 and A6).

Analysed in the same way as done in the validation study of Reuter et al. (2020), we find CO₂ biases with a station-to-station standard deviation of 0.57 ppm and an average scatter of 1.14 ppm (Fig. A5a). For CH₄, we find biases with a station-to-station standard deviation of 7.5 ppb and an average scatter of 10.6 ppb (Fig. A5b). Especially for XCO₂, these values are similar to values found for comparisons of satellite retrieval data products with TCCON (e.g. Reuter et al., 2020).



Appendix B: Filter variables and bias correction parameters

450 Tables A1 to A12 show the filter settings for the various GOSAT and GOSAT-2 products. Figs. A7 and A8 show the bias correction parameters and their relevance for GOSAT and GOSAT-2.

Author contributions. S. Noël adapted the FOCAL method to GOSAT and GOSAT-2, generated the updated FOCAL data products and performed the validation. M. Reuter developed the FOCAL method and provided the XCO₂ and XCH₄ reference databases and the TCCON validation tools. J. Borchardt provided the used python implementation for the SLIM XCO₂ and methane climatology. M. Hilker provided
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A. Di Noia and R. Parker provided the UoL, Y. Yoshida the NIES GOSAT data products.

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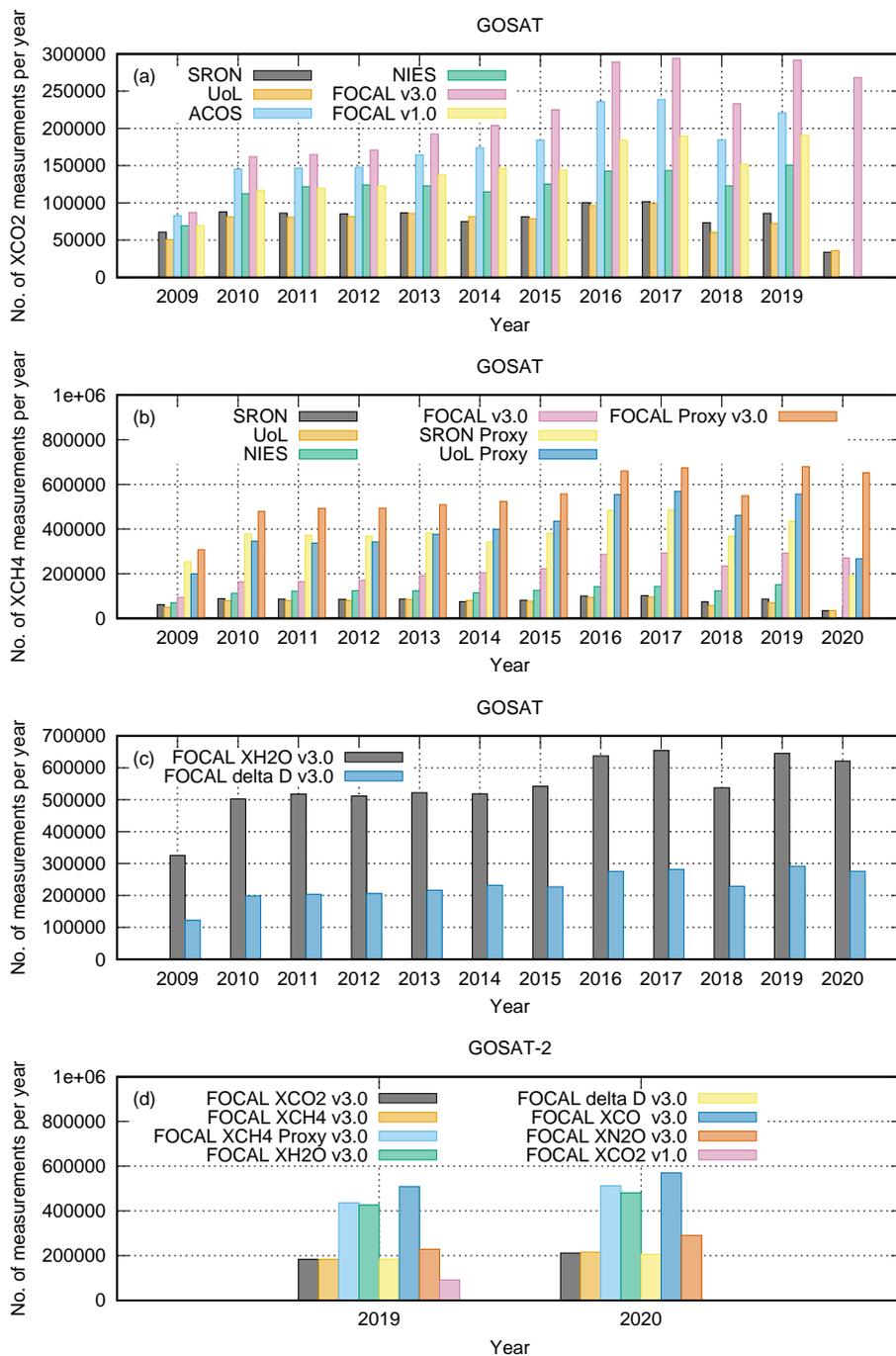


Figure 1. Number of GOSAT and GOSAT-2 data for different products as function of time (see Tab. 6 for details on version numbers). (a) GOSAT XCO₂. (b) GOSAT XCH₄. (c) GOSAT FOCAL XH₂O and δ D. (d) GOSAT-2 FOCAL products

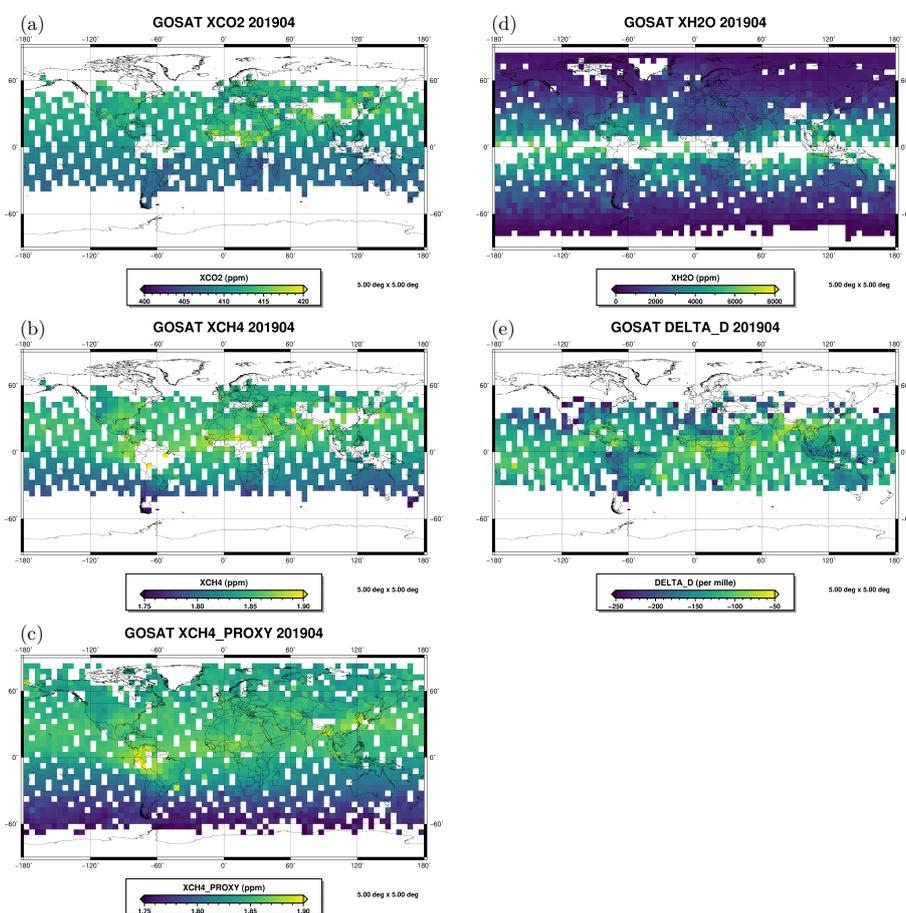


Figure 2. Maps of gridded GOSAT data for April 2019: (a) XCO₂. (b) XCH₄ full physics product. (c) XCH₄ proxy product. (d) XH₂O. (e) δD .

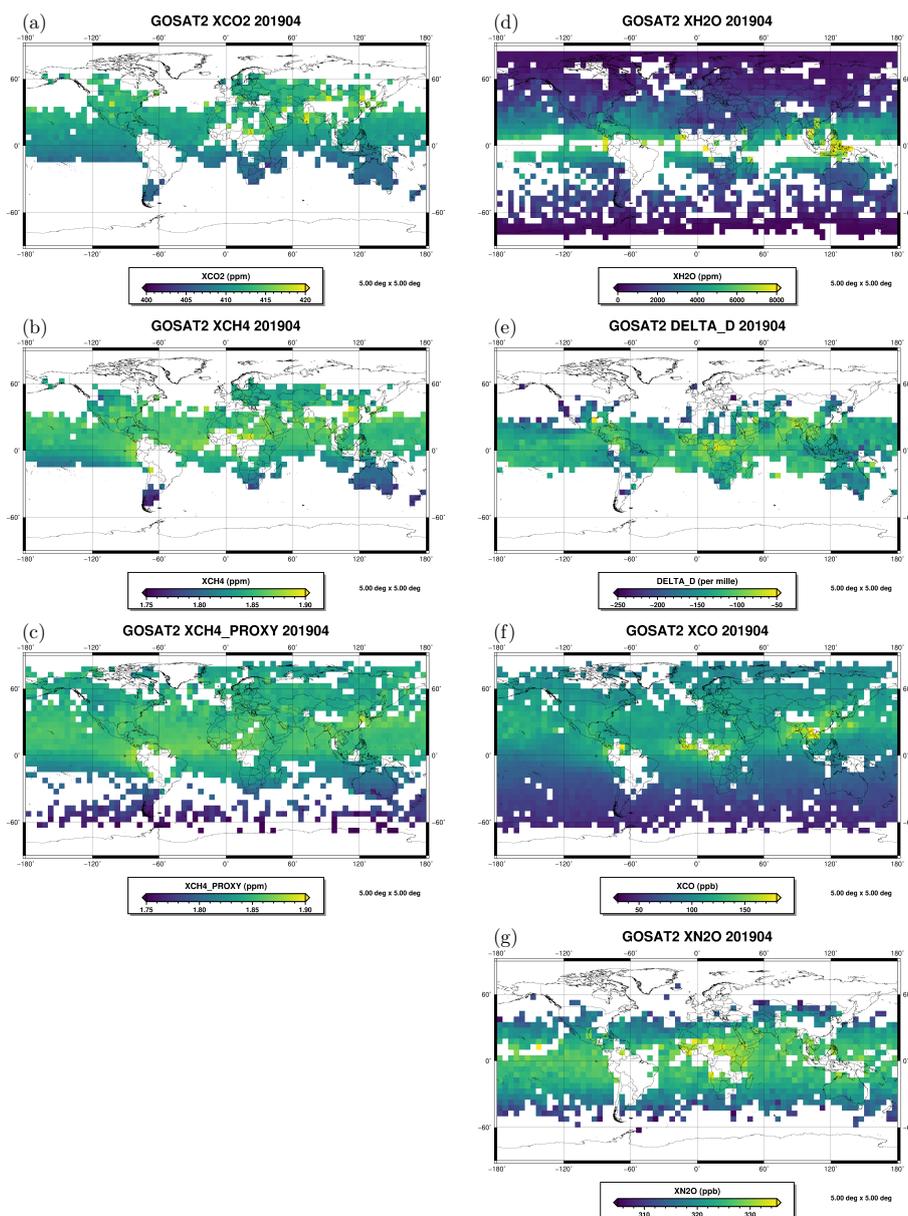


Figure 3. Maps of gridded GOSAT-2 data for April 2019: (a) XCO₂. (b) XCH₄ full physics product. (c) XCH₄ proxy product. (d) XH₂O. (e) δ D. (f) XCO. (g) XN₂O.

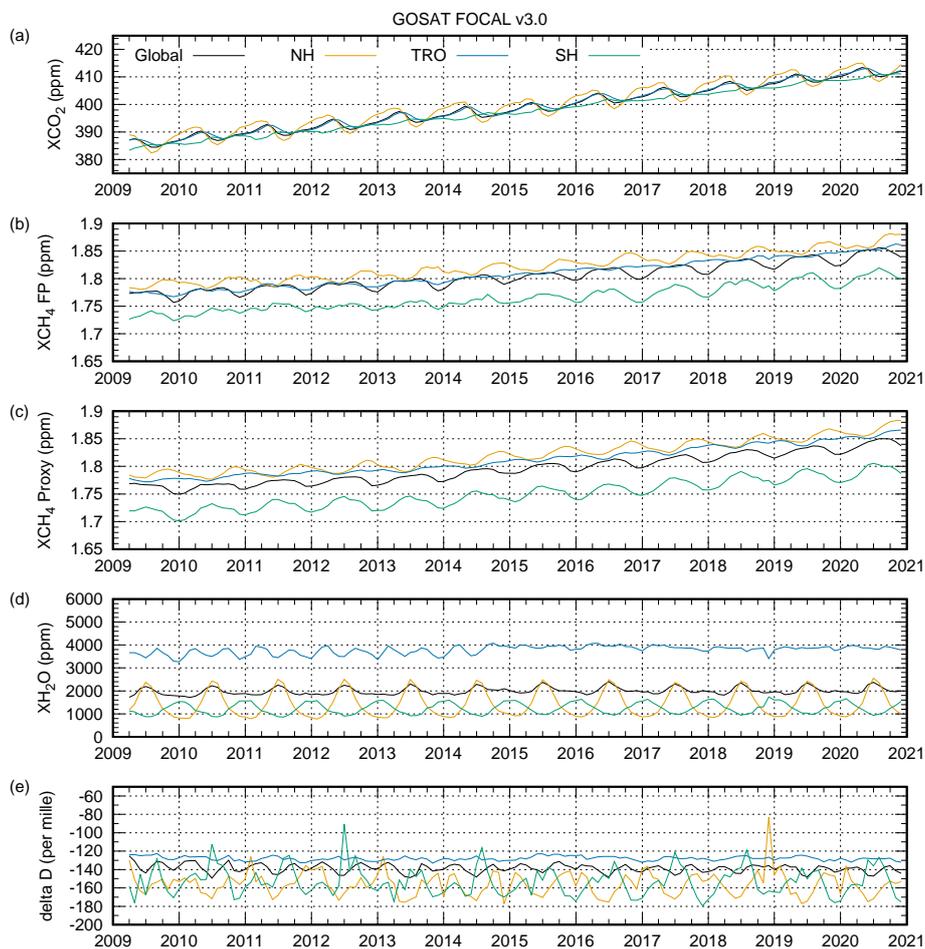


Figure 4. GOSAT time series. NH = Northern hemisphere ($> 25^{\circ}\text{N}$). TRO = Tropics ($25^{\circ}\text{S} - 25^{\circ}\text{N}$). SH = Southern hemisphere ($< 25^{\circ}\text{S}$). (a) XCO₂. (b) XCH₄ full physics product. (c) XCH₄ proxy product. (d) XH₂O. (e) δD .

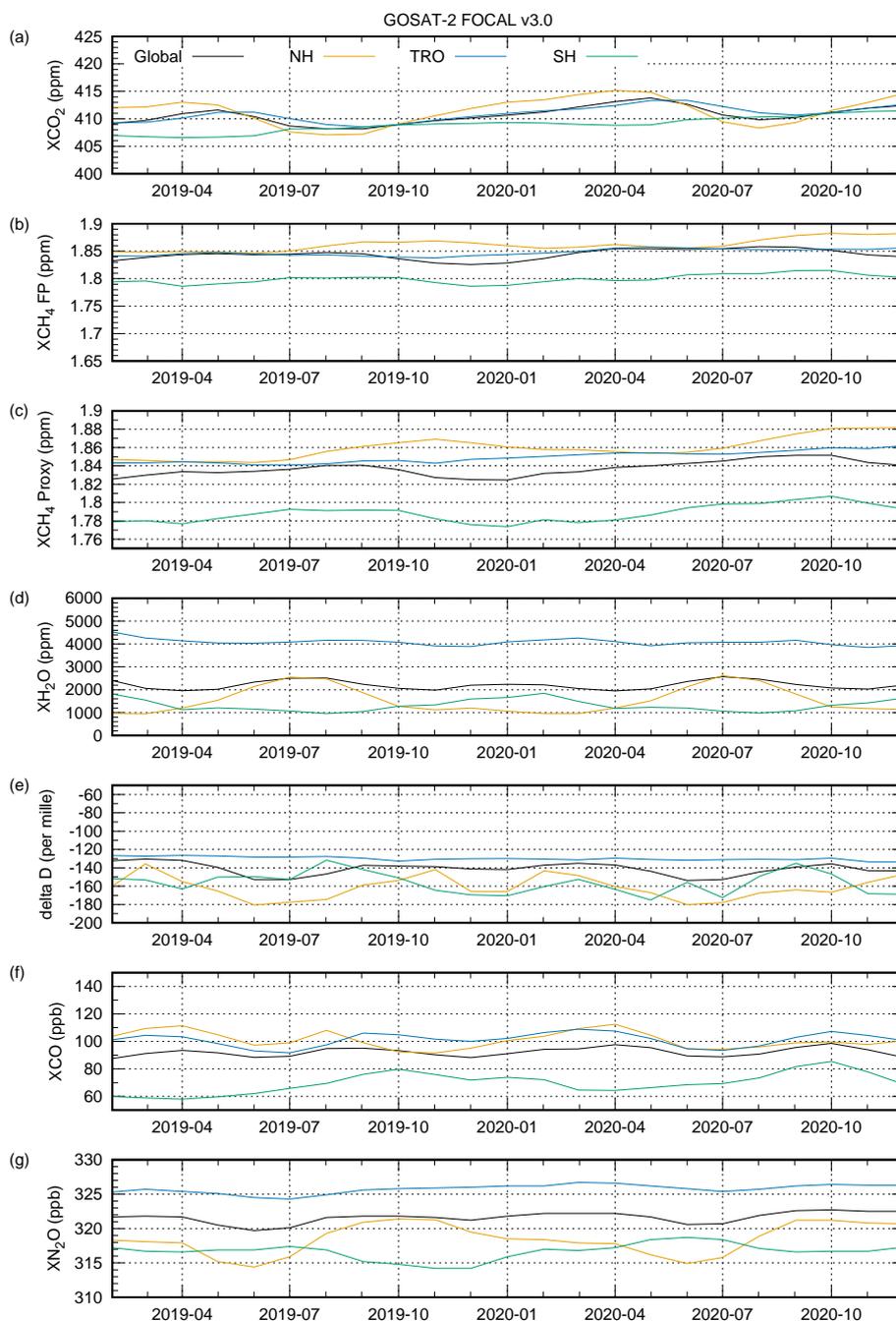


Figure 5. GOSAT-2 time series. NH = Northern hemisphere ($> 25^{\circ}\text{N}$). TRO = Tropics ($25^{\circ}\text{S} - 25^{\circ}\text{N}$). SH = Southern hemisphere ($< 25^{\circ}\text{S}$). (a) XCO_2 . (b) XCH_4 full physics product. (c) XCH_4 proxy product. (d) XH_2O . (e) δD . (f) XCO . (g) XN_2O .

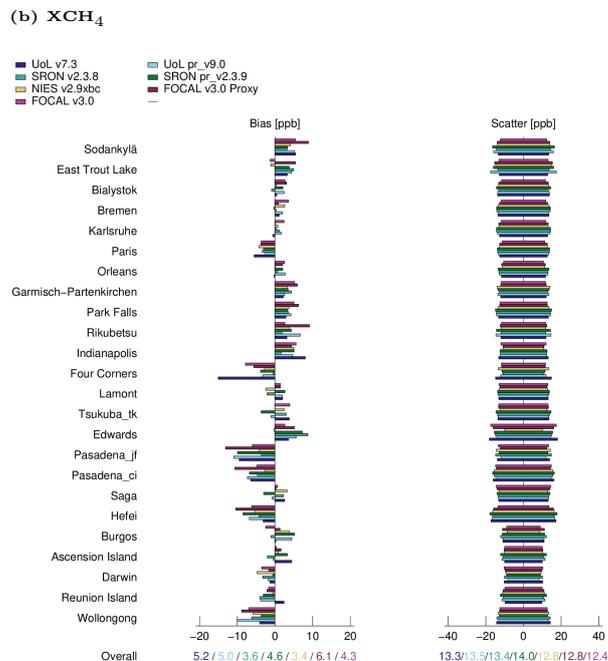
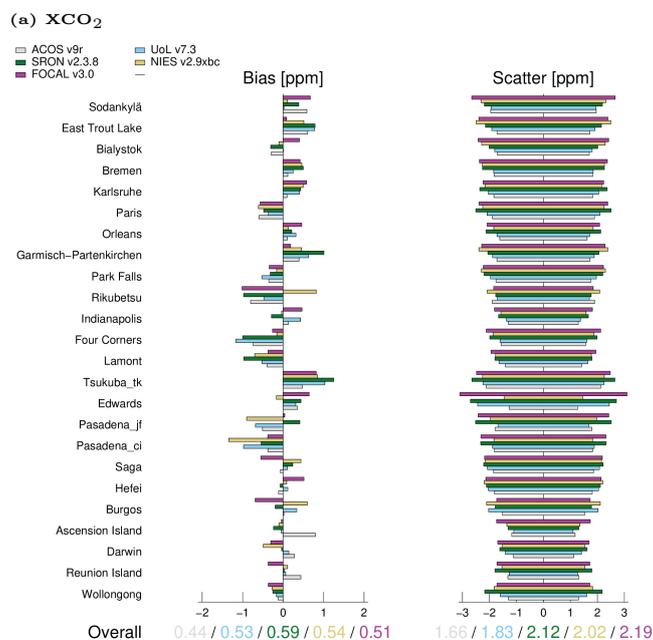
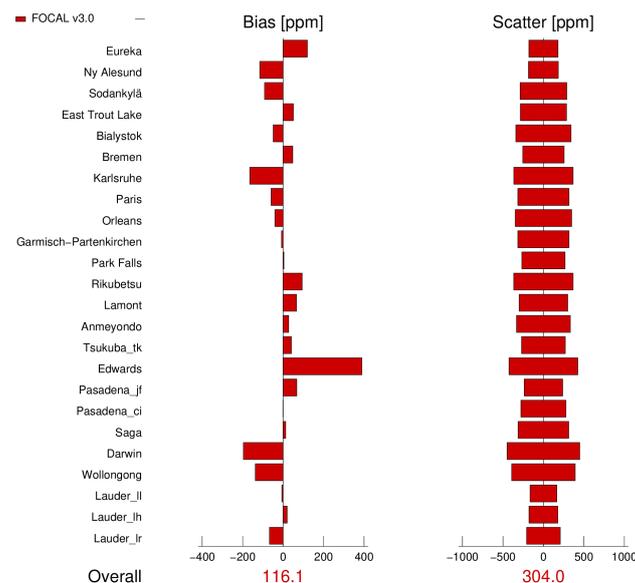


Figure 6. Overview of comparison results between different GOSAT products and TCCON data: Scatter and bias for different TCCON stations. Note that the mean station bias has been subtracted to better illustrate the local station differences. (c) XH_2O . (d) δD .



(a) XH_2O



(b) δD

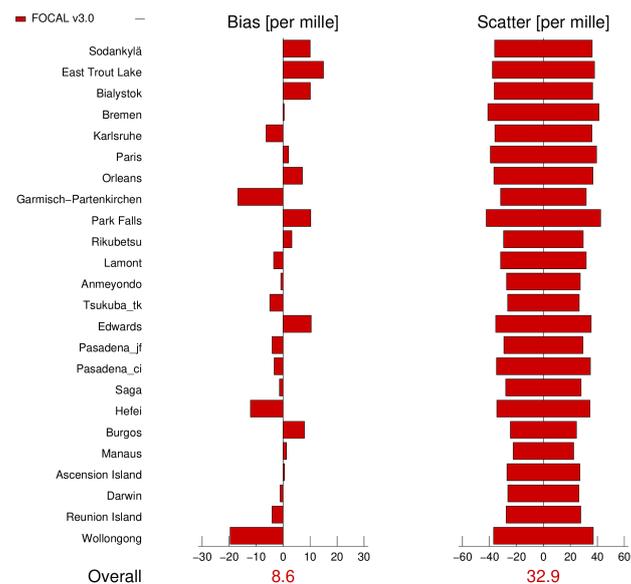
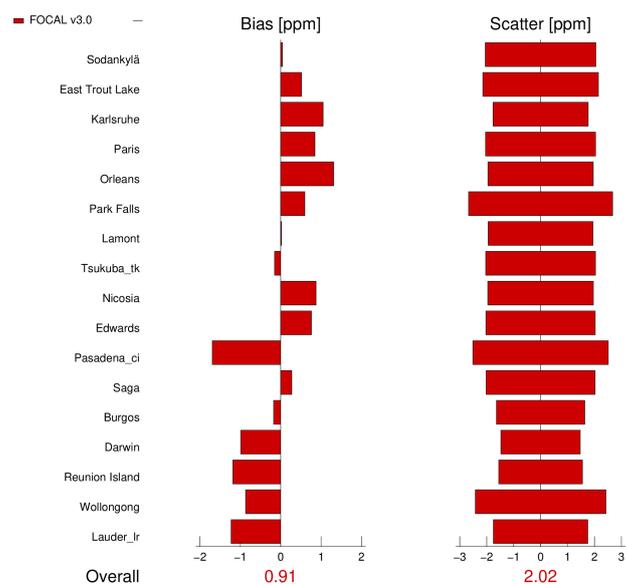


Figure 7. As Fig. 6, but for: (a) XH_2O . (b) δD .



(a) XCO₂



(b) XCH₄

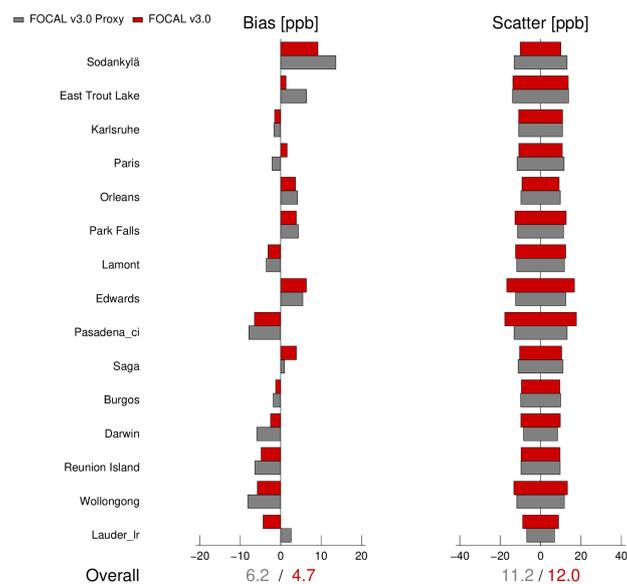
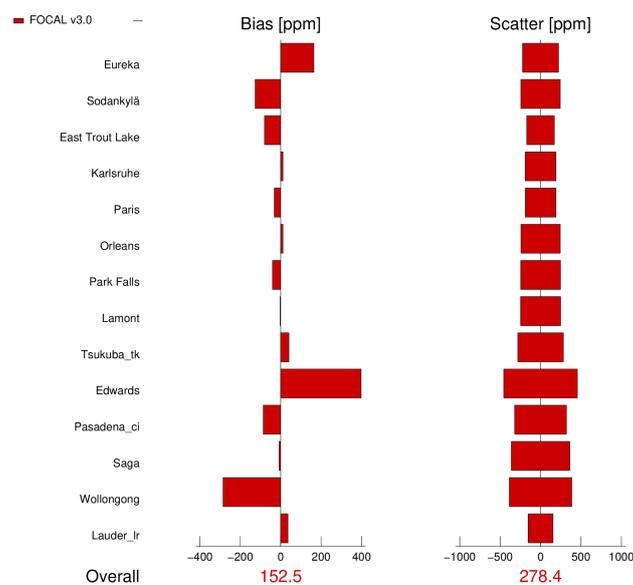


Figure 8. Overview of comparison results between GOSAT-2 FOCAL products and TCCON data: Scatter and bias for different TCCON stations. Note that the mean station bias has been subtracted to better illustrate the local station differences. (a) XCO₂. (b) XCH₄ (full physics and proxy products).



(a) XH_2O



(b) δD

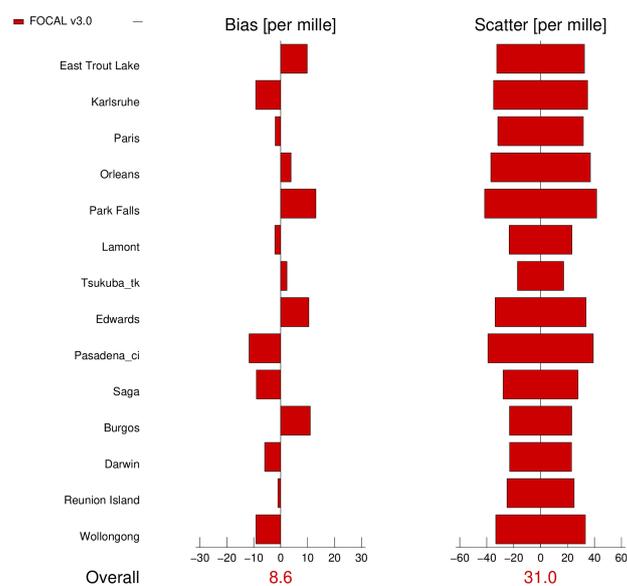
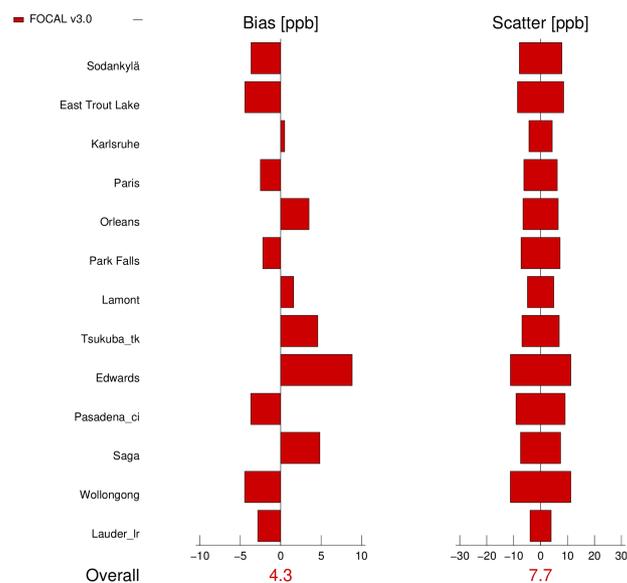


Figure 9. As Fig. 8, but for: (a) XH_2O . (b) δD .



(a) XCO



(b) XN₂O

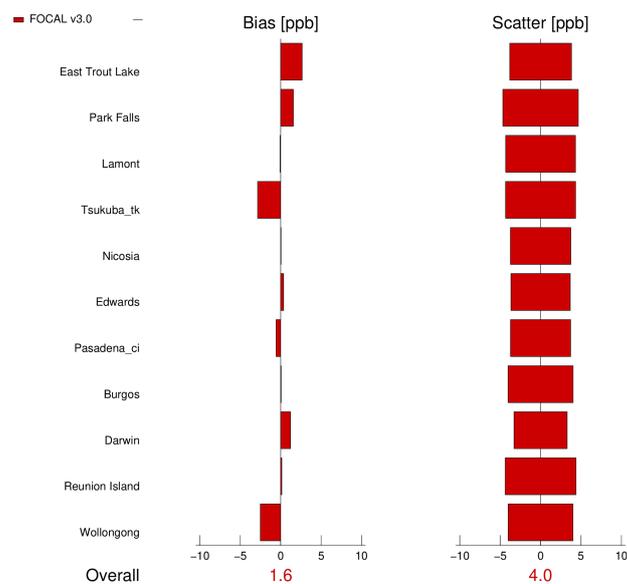


Figure 10. As Fig. 8, but for: (a) XCO. (b) XN₂O.

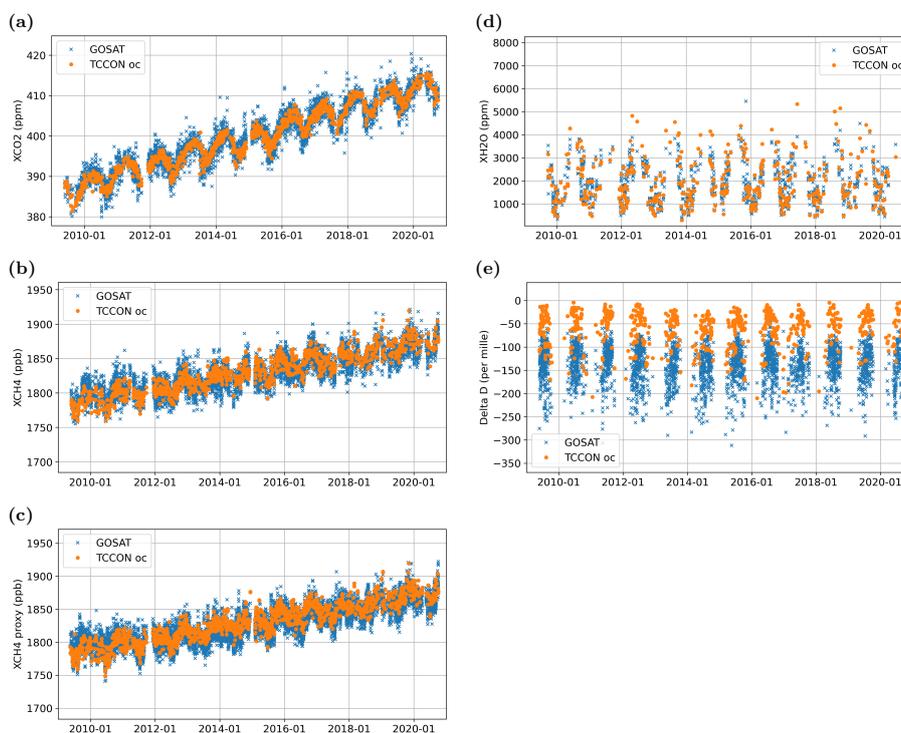


Figure 11. Example time series of TCCON and GOSAT FOCAL data at Lamont (station code oc). (a) XCO₂. (b) XCH₄ full physics product. (c) XCH₄ proxy product. (d) XH₂O. (e) δ D.

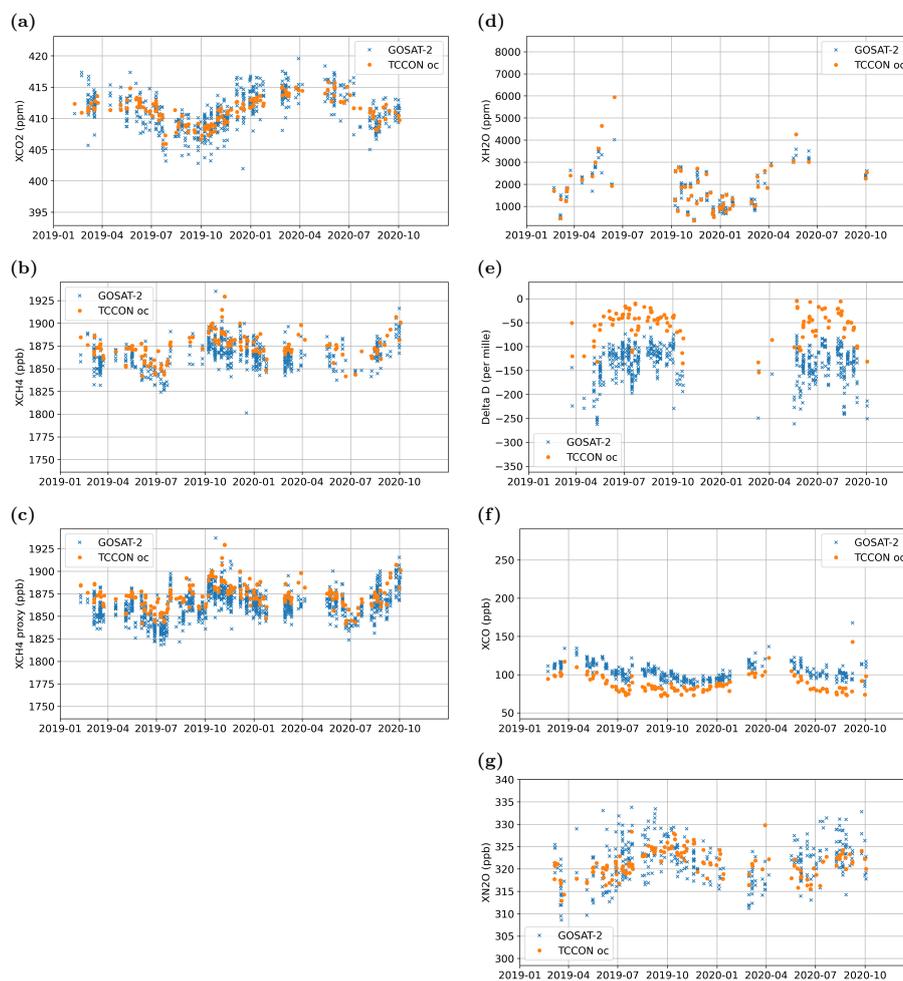


Figure 12. Example time series of TCCON and GOSAT-2 FOCAL data at Lamont (station code oc). (a) XCO₂. (b) XCH₄ full physics product. (c) XCH₄ proxy product. (d) XH₂O. (e) δD . (f) XCO. (g) XN₂O.



Table 1. TCCON stations used in this study (update of similar table in Noël et al. (2021)).

Site	Lon. (deg)	Lat. (deg)	Elev. (km)	Reference(s)
Anmeyondo (KR)	126.33	36.54	0.03	Goo et al. (2014)
Ascension Island (SH)	-14.33	-7.92	0.01	Feist et al. (2014)
Bialystok (PL)	23.03	53.23	0.18	Deutscher et al. (2019)
Bremen (DE)	8.85	53.10	0.04	Notholt et al. (2019a)
Burgos (PH)	120.65	18.53	0.04	Morino et al. (2018b)
Darwin (AU)	130.89	-12.42	0.03	Griffith et al. (2014a)
Edwards (US)	-117.88	34.96	0.70	Iraci et al. (2016a)
East Trout Lake (CA)	-104.99	54.35	0.50	Wunch et al. (2017)
Eureka (CA)	-86.42	80.05	0.61	Strong et al. (2019)
Four Corners (US)	-108.48	36.80	1.64	Dubey et al. (2014)
Garmisch-Partenkirchen (DE)	11.06	47.48	0.74	Sussmann and Rettinger (2018a)
Hefei (CN)	117.17	31.90	0.04	Liu et al. (2018)
Indianapolis (US)	-86.00	39.86	0.27	Iraci et al. (2016b)
Izaña (ES)	-16.50	28.30	2.37	Blumenstock et al. (2017)
Karlsruhe (DE)	8.43	49.10	0.11	Hase et al. (2014)
Lamont (US)	-97.49	36.60	0.32	Wennberg et al. (2016)
Lauder (NZ)	169.68	-45.04	0.37	Sherlock et al. (2014a, b) Pollard et al. (2019)
Nicosia (CY)	33.38	35.14	0.19	Petri et al. (2020)
Ny Ålesund (NO)	11.90	78.90	0.02	Notholt et al. (2019b)
Orleans (FR)	2.11	47.97	0.13	Warneke et al. (2019)
Paris (FR)	2.36	48.85	0.06	Te et al. (2014)
Park Falls (US)	-90.27	45.95	0.44	Wennberg et al. (2017)
Pasadena (US)	-118.13	34.13	0.21	Wennberg et al. (2015)
Reunion Island (FR)	55.49	-20.90	0.09	De Mazière et al. (2017)
Rikubetsu (JP)	143.77	43.46	0.36	Morino et al. (2017)
Saga (JP)	130.29	33.24	0.01	Kawakami et al. (2014)
Sodankylä (FI)	26.63	67.37	0.18	Kivi et al. (2014)
Tsukuba (JP)	140.12	36.05	0.03	Morino et al. (2018a)
Wollongong (AU)	150.88	-34.41	0.03	Griffith et al. (2014b)
Zugspitze (DE)	10.98	47.42	2.96	Sussmann and Rettinger (2018b)



Table 2. Definition of GOSAT/GOSAT-2 spectral fit windows (same for S and P). Windows 7 and 8 are only available for GOSAT-2. Cross sections are from HITRAN2016 except for those marked with “^a”, which are from ABSCO v5.1, and those marked with “^b”, which are from Gorshelev et al. (2014); Serdyuchenko et al. (2014).

No.	Primary target	Waveno. range (cm ⁻¹)	Considered gases
1	SIF	13170 – 13220	O ₂ ^a , H ₂ O ^a , O ₃ ^b
2	O ₂	12930 – 13170	O ₂ ^a , H ₂ O ^a , O ₃ ^b
3	HDO	6337 – 6410	CO ₂ , H ₂ O, HDO, CH ₄
4	CO ₂	6161 – 6297	CO ₂ ^a , H ₂ O, HDO, CH ₄
5	CH ₄	5945 – 6135	CO ₂ , H ₂ O, HDO, CH ₄
6	CO ₂	4801 – 4907	CO ₂ ^a , H ₂ O, HDO
7	N ₂ O	4364 – 4449	N ₂ O, H ₂ O, HDO, CH ₄
8	CO	4228 – 4328	CO, H ₂ O, HDO, CH ₄



Table 3. State vector elements and related retrieval settings. A priori values are also used as first guess. “Fit windows” lists the spectral windows (see Tab. 2) from which the element is determined. “each” means that a corresponding element is fitted in each fit window. A priori values labelled as “PP” are taken from pre-processing; “est.” denotes that they have been estimated from the background signal.

Element	Fit windows	A priori	A priori uncertainty	Comment
Gases				
co2_lay	3,4,5,6 (S&P)	PP	10.0	CO ₂ profile (5 layers), in ppm
ch4_lay	3,4,5 (S&P)	PP	0.045	CH ₄ profile (5 layers), in ppm
h2o_lay	3,4,5,6 (S&P)	PP	5.0	H ₂ O profile (5 layers), in ppm
sif_fac	1 (S&P)	0.	5.	SIF spectrum scaling factor
delta_d	3,4,5,6 (S&P)	-200.	1000.	δD profile scaling factor
n2o_scl	7 (S&P)	1.	0.1	N ₂ O profile scaling factor, only GOSAT-2
co_scl	8 (S&P)	1.	1.0	CO profile scaling factor, only GOSAT-2
Scattering parameters				
pre_sca_s	1–6 S	0.2	1.	Layer height (pressure), S
tau_sca_0_s	1–6 S	0.01	0.1	Optical depth, S
ang_sca_s	1–6 S	4.0	1.	Ångström coefficient, S
pre_sca_p	1–6 P	0.2	1.	Layer height (pressure), P
tau_sca_0_p	1–6 P	0.01	0.1	Optical depth, P
ang_sca_p	1–6 P	4.0	1.	Ångström coefficient, P
Polynomial coefficients (surface albedo)				
poly0	each	est.	0.1	estimated surface albedo
poly1	each	0.0	0.01	
poly2	each	0.0	0.01	not in SIF window (1)
poly3	each	0.0	0.01	not in SIF window (1)
poly4	each	0.0	0.01	only in N ₂ O window (7)
Spectral corrections				
wav_shi	each	0.0	0.1	Wavenumber shift
wav_squ	each	0.0	0.001	Wavenumber squeeze



Table 4. Filter settings for all products. “–” denotes that no limit is applied.

Gas	SZA Filter	P_{τ}	P_V
Land			
XCO ₂	75°	40%	50%
XCH ₄	75°	40%	50%
XCH ₄ Proxy	75°	–	20%
XH ₂ O	–	–	30%
δ D	75°	40%	50%
XN ₂ O	75°	40%	50%
XCO	75°	–	20%
Water			
XCO ₂	75°	40%	40%
XCH ₄	75°	40%	40%
XCH ₄ Proxy	75°	–	20%
XH ₂ O	–	–	30%
δ D	75°	40%	40%
XN ₂ O	75°	40%	40%
XCO	75°	–	20%



Table 5. Coefficients of linear uncertainty correction.

Gas	Surface	Offset (ppm)	Slope
GOSAT			
XCO ₂	land	1.030937	1.27
XCO ₂	water	0.568207	0.83
XCH ₄	land	0.002487	2.07
XCH ₄	water	0.005121	0.83
XCH ₄ Propy	land	0.007951	0.67
XCH ₄ Proxy	water	0.006026	0.59
GOSAT-2			
XCO ₂	land	0.292586	2.27
XCO ₂	water	0.596544	0.77
XCH ₄	land	0.004791	2.02
XCH ₄	water	0.006171	0.60
XCH ₄ Propy	land	0.008328	0.58
XCH ₄ Proxy	water	0.006286	0.53



Table 6. Results from TCCON comparisons. N_{stations} denotes the number of TCCON stations involved in the comparison, N_{data} is the number of collocated data points. All products are full physics products except for those marked as ‘Proxy’.

Product (unit)	N_{stations}	N_{data}	Mean station bias	Station-to-station bias	Mean scatter	Seasonal bias
GOSAT 2009–2020 XCO ₂ products vs. TCCON						
ACOS v9r (ppm)	24	35827	0.08	0.44	1.66	0.34
UoL v7.3 (ppm)	24	24223	0.21	0.53	1.83	0.39
SRON v2.3.8 (ppm)	24	22907	0.41	0.59	2.12	0.40
NIES v02.9xbc (ppm)	24	31323	0.61	0.54	2.02	0.40
FOCAL v3.0 (ppm)	24	32505	0.40	0.51	2.19	0.33
GOSAT 2009–2020 XCH ₄ products vs. TCCON						
UoL v7.3 (ppb)	24	23661	-1.89	5.15	13.33	3.57
UoL Proxy v9.0 (ppb)	24	72849	-0.78	4.97	13.46	3.01
SRON v2.3.8 (ppb)	24	22907	3.24	3.64	13.39	2.92
SRON Proxy v2.3.9 (ppb)	24	74615	1.34	4.60	13.96	2.62
NIES v02.9xbc (ppb)	24	31334	-0.61	3.38	12.76	2.87
FOCAL v3.0 (ppb)	24	30245	-3.04	4.28	12.37	2.83
FOCAL v3.0 Proxy (ppb)	24	72954	-4.75	6.11	12.84	2.52
GOSAT 2009–2020 FOCAL v3.0 water vapour products vs. TCCON						
XH ₂ O (ppm)	24	19739	-78.82	116.13	304.05	65.79
δD (‰)	24	21892	-83.41	8.62	32.95	6.29
GOSAT-2 2019–2020 FOCAL v3.0 products vs. TCCON						
XCO ₂ (ppm)	17	5251	-0.01	0.91	2.02	0.62
XCH ₄ (ppb)	15	4400	-6.61	4.71	12.00	2.45
XCH ₄ Proxy ^a (ppb)	15	10370	-6.02	6.15	11.19	3.05
XH ₂ O (ppm)	14	3500	-20.89	152.47	278.41	109.91
δD (‰)	14	2762	-82.76	8.55	31.00	12.69
XCO (ppb)	13	3777	14.80	4.32	7.67	2.84
XN ₂ O (ppb)	11	3151	0.63	1.61	4.02	1.56

^aXCH₄ Proxy validated together with full physics product, i.e. for same subset of TCCON stations

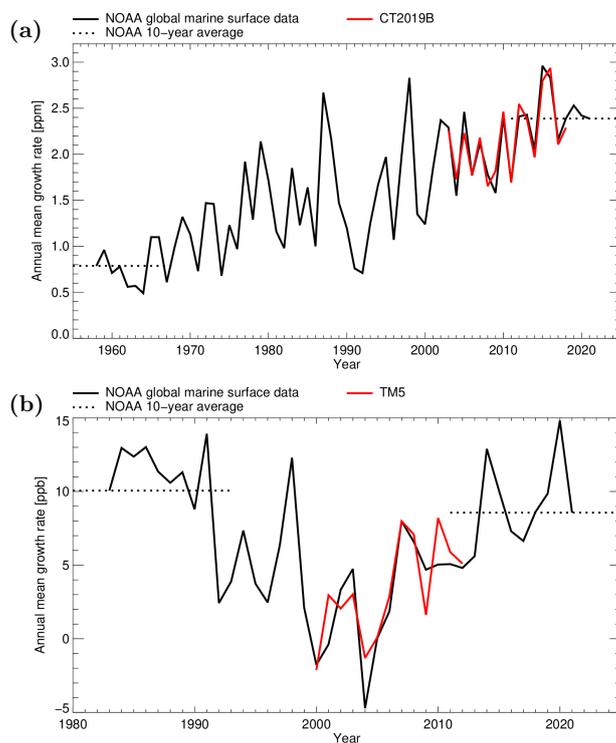


Figure A1. Global growth rates for CO₂ (a) and CH₄ (b).

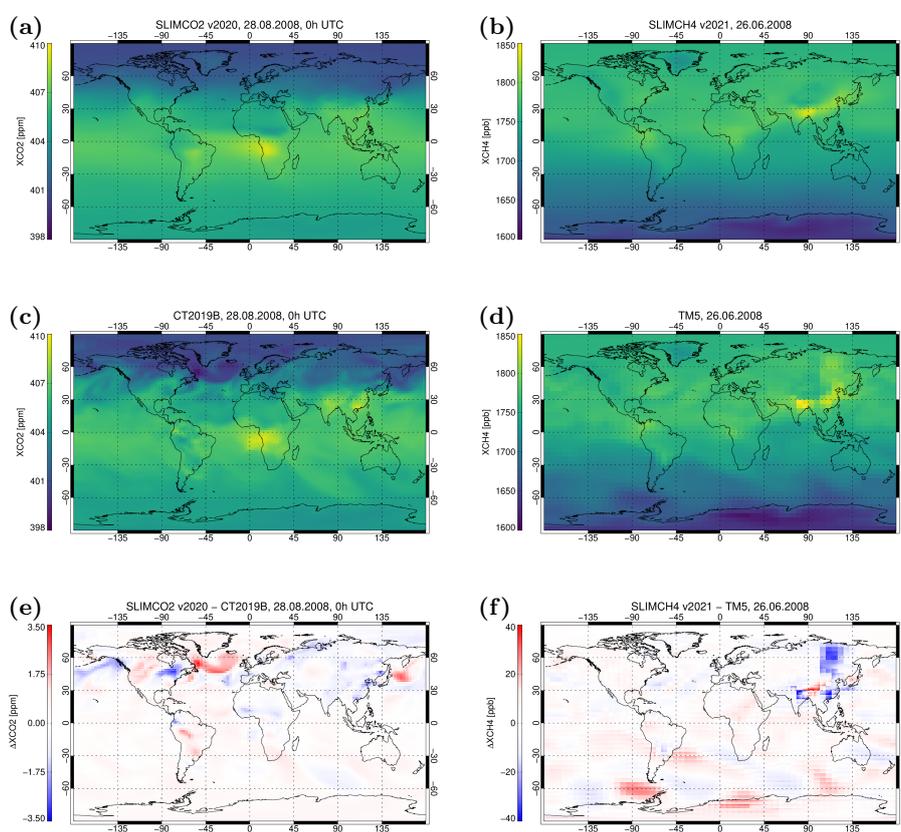


Figure A2. Example Maps of SLIMCO₂ (a) and SLIMCH₄ (b) data. Panels (c) and (d) show corresponding data from the underlying models (CT2019B, TM5). The differences between the SLIM results and these model data are shown in panels (e) and (f).

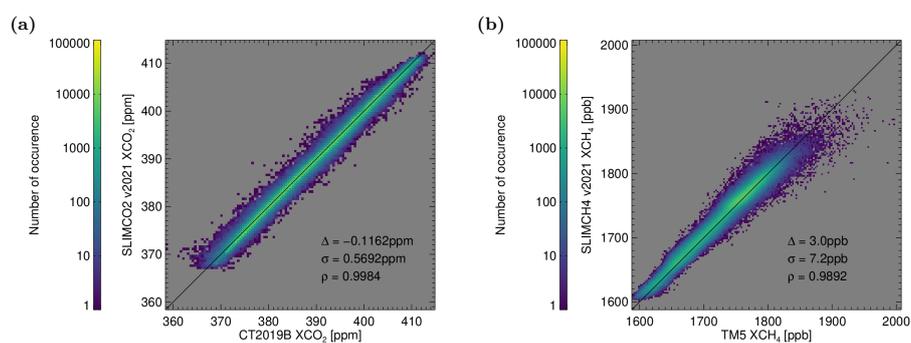


Figure A3. Scatter plot of the data shown in Fig. A2. (a) SLIMCO2 data vs. CT2019B. (b) SLIMCH4 vs. TM5. σ corresponds to the standard deviation of the difference δ corresponds to the average bias, and ρ is the Pearson correlation coefficient.

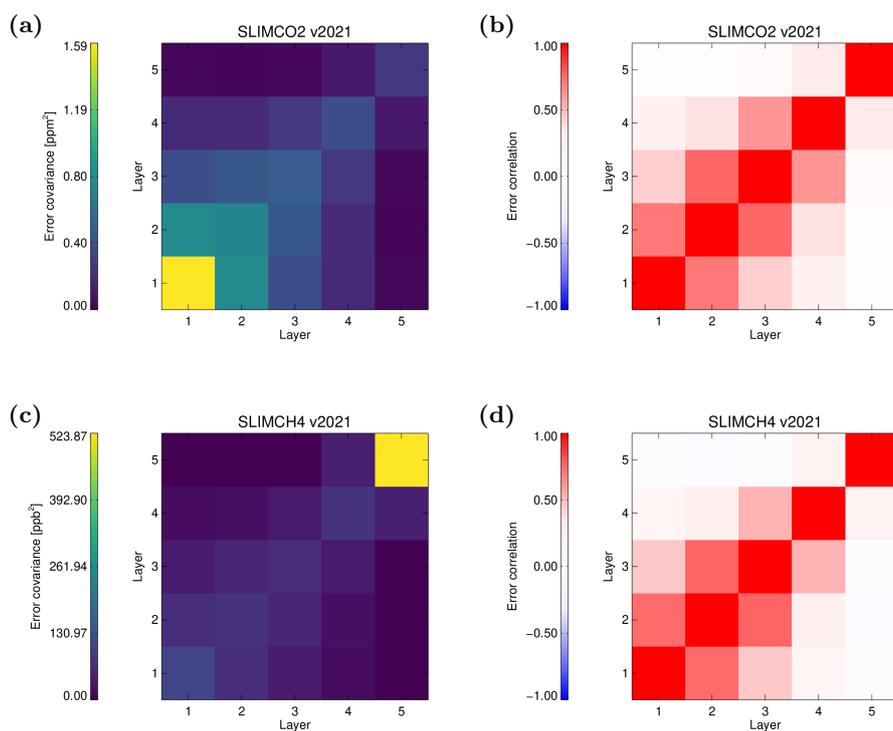


Figure A4. Error covariance matrices for SLIMCO2 (a) and SLIMCH4(c) and corresponding error correlation matrices (b, d).

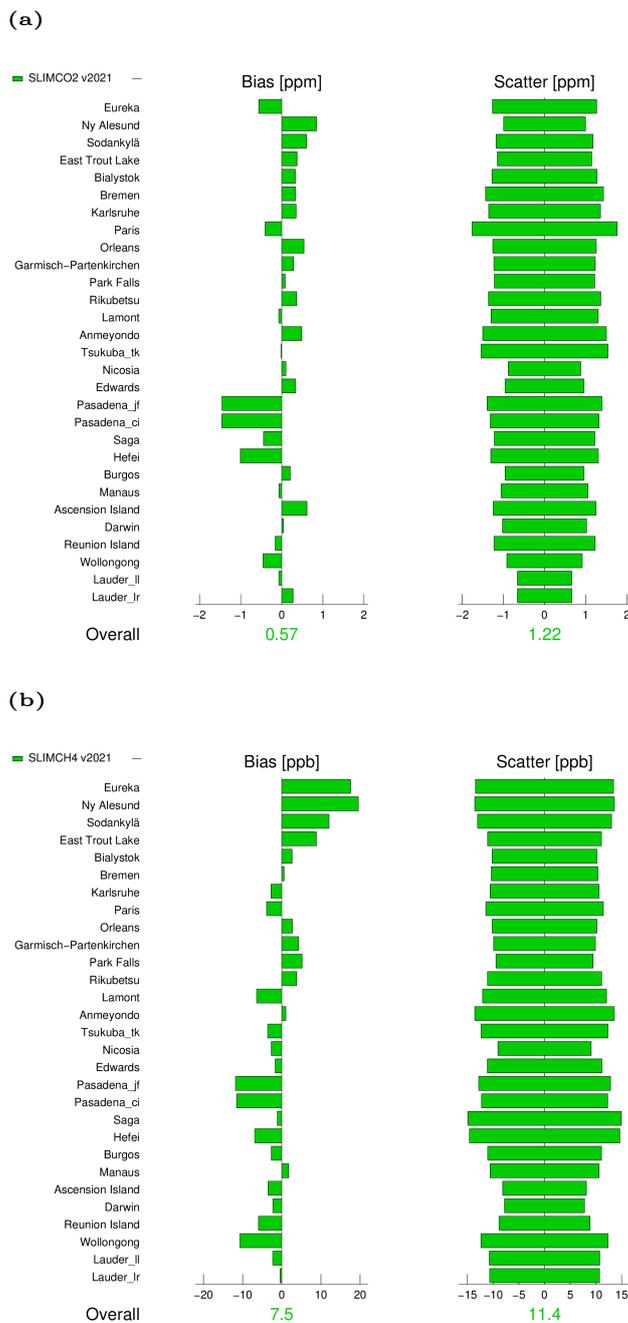


Figure A5. Overview of TCCON validation results for SLIMCO2 (a) and SLIMCH4 (b). The mean station bias has been subtracted to better illustrate the local station differences.

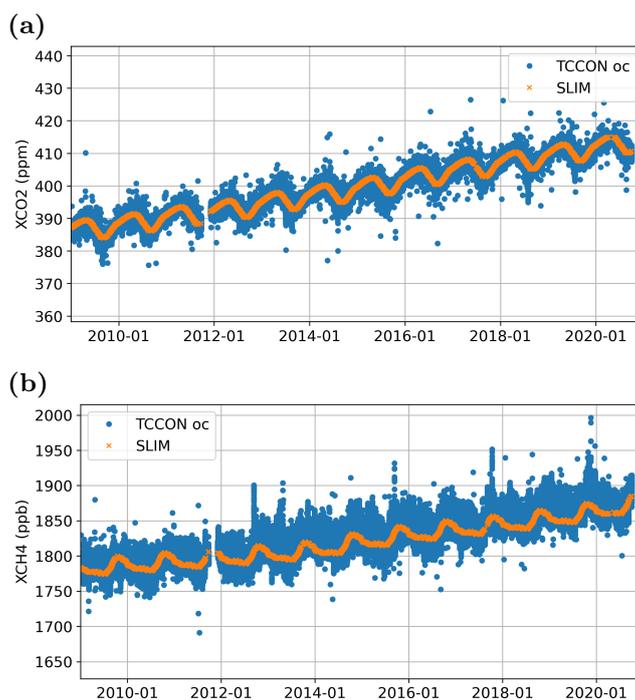


Figure A6. Time series of XCO₂ (a) and XCH₄ (b) from TCCON and SLIM at Lamont (station code oc).

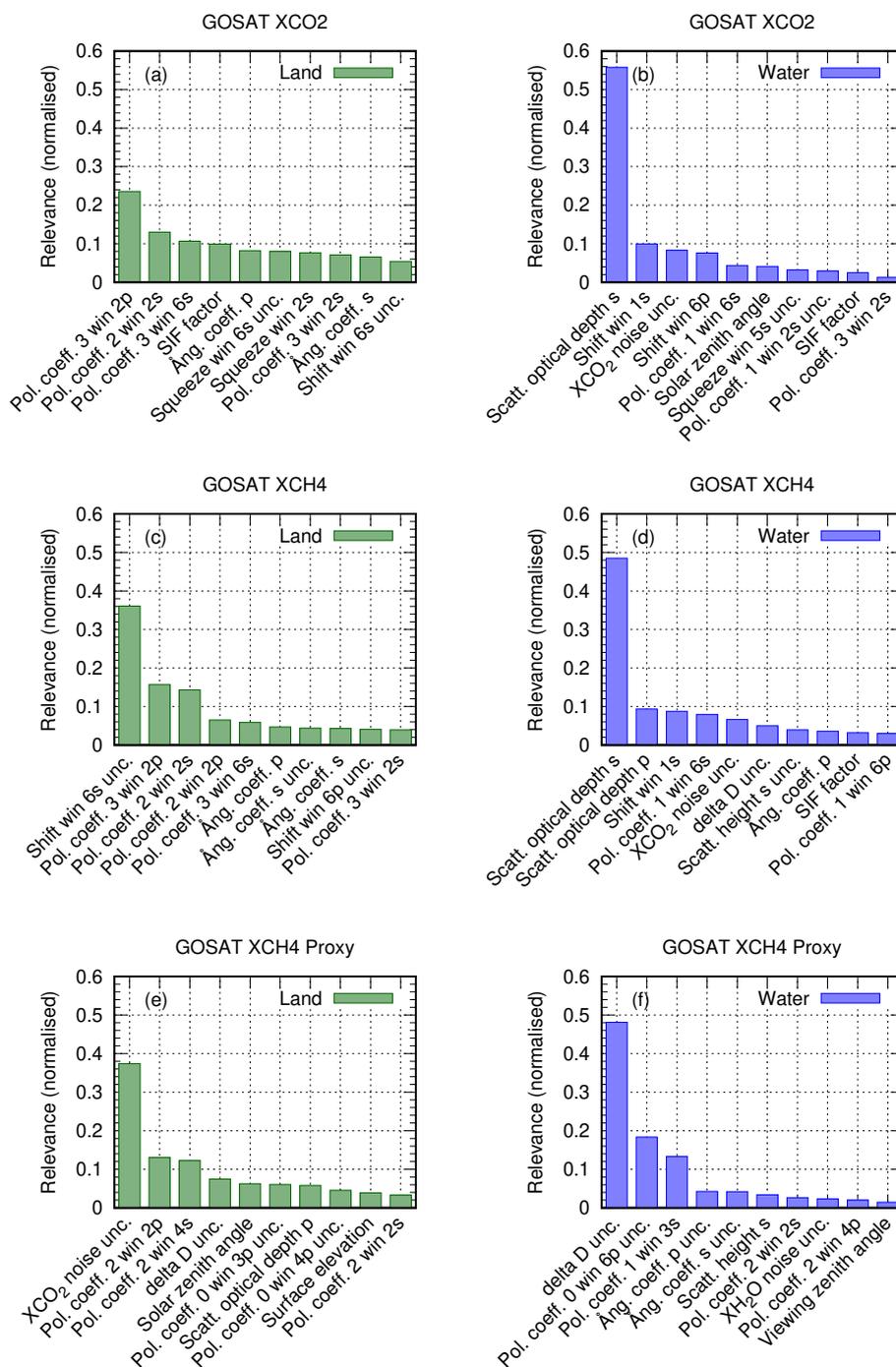


Figure A7. Variables selected for the GOSAT random forest bias correction and their relevance. Top: XCO₂. Middle: XCH₄. Bottom: XCH₄ Proxy. Left/right: For land/water surface.

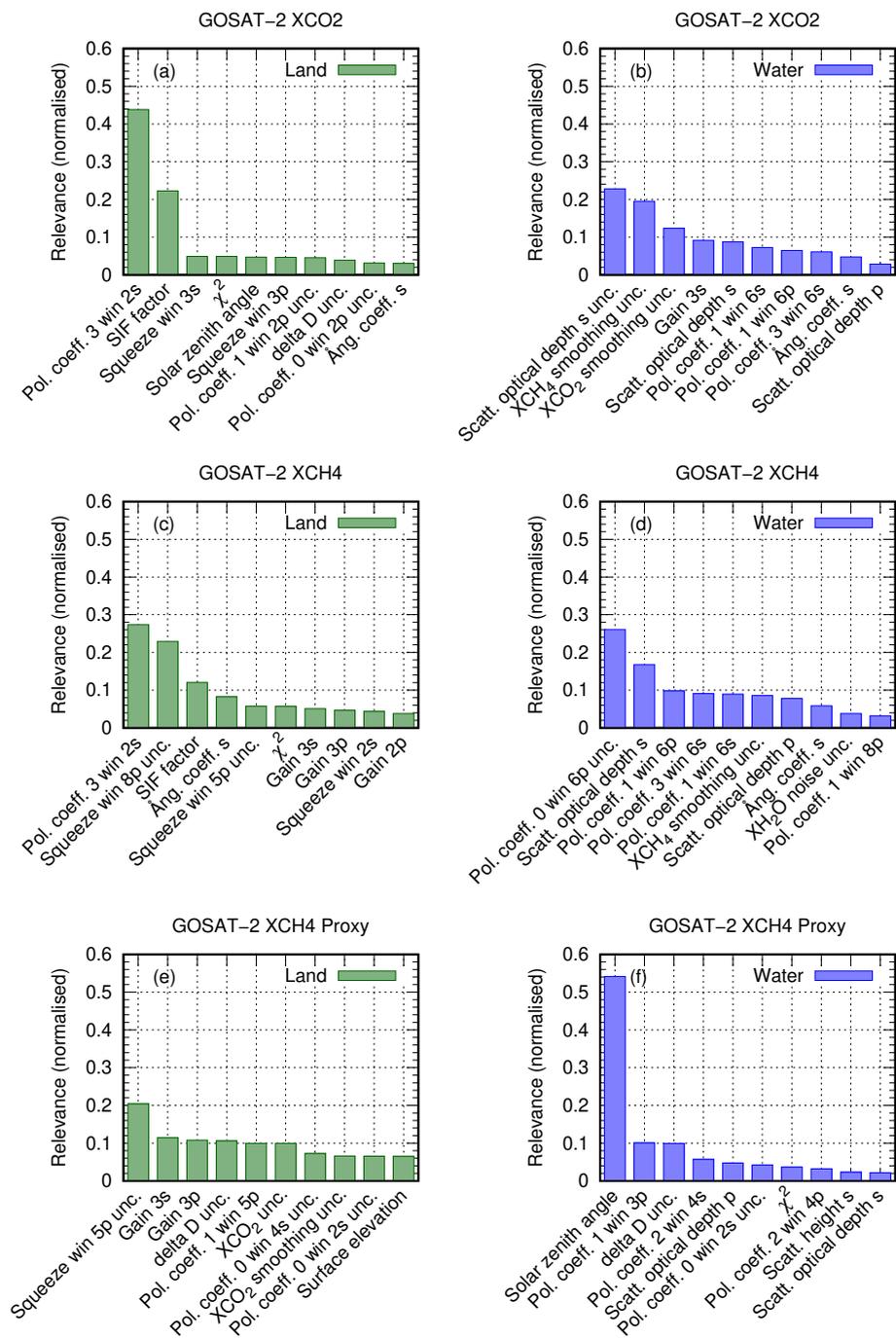


Figure A8. Same as Fig. A7, but for GOSAT-2.



Table A1. XCO₂ filter variables and limits for GOSAT. “–” means that no limit is applied.

Land			Water		
Variable	valid range		Variable	valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. optical depth s	$1.09 \cdot 10^{-3}$	$5.37 \cdot 10^{-2}$	Scatt. optical depth p	$-7.28 \cdot 10^{-2}$	$3.53 \cdot 10^{-2}$
Scatt. optical depth p	$-5.09 \cdot 10^{-3}$	$2.80 \cdot 10^{-2}$	Scatt. optical depth s	$4.40 \cdot 10^{-3}$	$5.76 \cdot 10^{-2}$
Pol. coeff. 3 win 2s	$-6.98 \cdot 10^{-3}$	$-6.42 \cdot 10^{-5}$	Pol. coeff. 3 win 2s	–	$1.87 \cdot 10^{-3}$
Pol. coeff. 3 win 2p	$-7.32 \cdot 10^{-3}$	$2.91 \cdot 10^{-4}$	XCO ₂ noise unc. (ppm)	0.58	1.45
Surface roughness (m)	–	54.00	Pol. coeff. 1 win 6p	$2.66 \cdot 10^{-4}$	–
XCH ₄ noise unc. (ppm)	$3.89 \cdot 10^{-3}$	$6.58 \cdot 10^{-3}$	Pol. coeff. 1 win 5p	$8.01 \cdot 10^{-4}$	–
Scatt. Ångström coeff. p	1.07	–	Pol. coeff. 1 win 5s	$7.67 \cdot 10^{-5}$	–
Spectral squeeze win 3p	$-1.20 \cdot 10^{-3}$	$1.21 \cdot 10^{-3}$	Pol. coeff. 0 win 3s unc.	–	$3.05 \cdot 10^{-4}$
Pol. coeff. 1 win 4s	$-1.46 \cdot 10^{-2}$	$-3.05 \cdot 10^{-3}$	Pol. coeff. 0 win 4p unc.	–	$4.50 \cdot 10^{-4}$
Spectral squeeze win 3s	$-1.21 \cdot 10^{-3}$	$1.24 \cdot 10^{-3}$	δD unc. (per mille)	–	391.41
Pol. coeff. 1 win 6s	$-3.62 \cdot 10^{-3}$	–	Pol. coeff. 0 win 5s unc.	–	$5.72 \cdot 10^{-4}$
Scatt. Ångström coeff. s	$-8.71 \cdot 10^{-2}$	–	χ ²	–	1.02



Table A2. XCH₄ filter variables and limits for GOSAT. “–” means that no limit is applied.

Variable	Land		Variable	Water	
	valid range			valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. optical depth s	$-6.59 \cdot 10^{-3}$	$3.45 \cdot 10^{-2}$	Scatt. optical depth p	$-7.28 \cdot 10^{-2}$	$3.52 \cdot 10^{-2}$
Scatt. optical depth p	$2.00 \cdot 10^{-3}$	$2.80 \cdot 10^{-2}$	Scatt. optical depth s	$4.40 \cdot 10^{-3}$	$7.55 \cdot 10^{-2}$
Pol. coeff. 3 win 2p	$-7.32 \cdot 10^{-3}$	$4.12 \cdot 10^{-4}$	Pol. coeff. 3 win 2p	$-8.80 \cdot 10^{-3}$	$9.59 \cdot 10^{-5}$
Scatt. Ångström coeff. p unc.	0.16	–	Pol. coeff. 1 win 5p	$7.97 \cdot 10^{-4}$	–
Surface roughness (m)	–	55.00	Pol. coeff. 1 win 6p	$2.23 \cdot 10^{-4}$	$4.51 \cdot 10^{-3}$
Pol. coeff. 3 win 2s	$-6.98 \cdot 10^{-3}$	$4.90 \cdot 10^{-4}$	Pol. coeff. 0 win 2p unc.	–	$5.32 \cdot 10^{-4}$
Pol. coeff. 1 win 4p	–	$-4.85 \cdot 10^{-3}$	Pol. coeff. 1 win 5s	$4.26 \cdot 10^{-5}$	–
Pol. coeff. 1 win 4s	$-1.46 \cdot 10^{-2}$	$-4.99 \cdot 10^{-3}$	Pol. coeff. 0 win 5p unc.	$5.98 \cdot 10^{-5}$	$3.61 \cdot 10^{-4}$
Spectral squeeze win 5s unc.	$2.02 \cdot 10^{-4}$	$3.99 \cdot 10^{-4}$	Pol. coeff. 0 win 3s unc.	–	$2.63 \cdot 10^{-4}$
Pol. coeff. 1 win 6s	$-3.79 \cdot 10^{-3}$	–	XCO ₂ noise unc. (ppm)	0.58	1.47
Scatt. Ångström coeff. s unc.	0.14	1.00	Pol. coeff. 0 win 5s unc.	–	$5.88 \cdot 10^{-4}$
Spectral squeeze win 3p	$-1.50 \cdot 10^{-3}$	$1.61 \cdot 10^{-3}$	Pol. coeff. 1 win 6s	$4.83 \cdot 10^{-5}$	$4.53 \cdot 10^{-3}$



Table A3. XCH₄ Proxy filter variables and limits for GOSAT. “–” means that no limit is applied.

Variable	Land		Variable	Water	
	valid range			valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Pol. coeff. 1 win 4s	–	$-4.11 \cdot 10^{-3}$	XCO ₂ smoothing unc. (ppm)	–	1.21
XH ₂ O noise unc. (ppm)	–	20.08	Spectral shift win 3p unc.	–	$1.29 \cdot 10^{-3}$
XCH ₄ noise unc. (ppm)	–	$1.48 \cdot 10^{-2}$	XCO ₂ unc. (ppm)	–	5.14
χ^2	–	0.97	XCO ₂ noise unc. (ppm)	–	2.40
Spectral squeeze win 5s unc.	–	$5.93 \cdot 10^{-4}$	Pol. coeff. 0 win 4p unc.	$7.16 \cdot 10^{-5}$	$5.98 \cdot 10^{-4}$
Scatt. optical depth p	-0.24	0.13	Pol. coeff. 2 win 4p	–	$1.00 \cdot 10^{-4}$
Spectral squeeze win 3p	–	$1.67 \cdot 10^{-3}$	Pol. coeff. 0 win 2s	$3.64 \cdot 10^{-2}$	–
Pol. coeff. 0 win 6p unc.	–	$1.04 \cdot 10^{-3}$	δD unc. (per mille)	–	183.57
Pol. coeff. 1 win 2p	$-7.56 \cdot 10^{-3}$	$4.48 \cdot 10^{-2}$	Scatt. Ångström coeff. s unc.	$4.11 \cdot 10^{-2}$	1.00
Pol. coeff. 1 win 4p	–	$-3.95 \cdot 10^{-3}$			



Table A4. XH₂O filter variables and limits for GOSAT. “–” means that no limit is applied.

Land			Water		
Variable	valid range		Variable	valid range	
	min.	max.		min.	max.
δD unc. (per mille)	26.77	–	δD unc. (per mille)	21.29	–
Spectral squeeze win 2p unc.	$6.25 \cdot 10^{-4}$	–	XH ₂ O noise unc. (ppm)	–	30.47
Pol. coeff. 2 win 6p unc.	$7.21 \cdot 10^{-5}$	–	Pol. coeff. 0 win 6p unc.	$1.61 \cdot 10^{-4}$	–
Pol. coeff. 0 win 2s unc.	$1.34 \cdot 10^{-4}$	–			
Pol. coeff. 0 win 5p unc.	$8.71 \cdot 10^{-5}$	–			



Table A5. δD filter variables and limits for GOSAT. “–” means that no limit is applied.

Land			Water		
Variable	valid range		Variable	valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. optical depth s	$1.37 \cdot 10^{-2}$	–	Scatt. optical depth s	$1.34 \cdot 10^{-2}$	$6.77 \cdot 10^{-2}$
δD unc. (per mille)	–	36.02	Scatt. optical depth p	$1.48 \cdot 10^{-2}$	$6.18 \cdot 10^{-2}$
XH ₂ O noise unc. (ppm)	7.27	62.48	δD unc. (per mille)	–	38.89
XH ₂ O unc. (ppm)	8.25	64.63	XH ₂ O noise unc. (ppm)	9.29	104.62
SIF factor unc.	0.43	–	Pol. coeff. 1 win 1p unc.	$3.22 \cdot 10^{-4}$	$1.09 \cdot 10^{-3}$
Pol. coeff. 1 win 6p	$-9.43 \cdot 10^{-3}$	$1.65 \cdot 10^{-2}$	Pol. coeff. 1 win 6s	$-9.81 \cdot 10^{-3}$	$3.66 \cdot 10^{-3}$
Spectral squeeze win 2s unc.	$3.58 \cdot 10^{-4}$	$6.12 \cdot 10^{-4}$	Pol. coeff. 1 win 6p	$-3.13 \cdot 10^{-3}$	$3.58 \cdot 10^{-3}$



Table A6. XCO₂ filter variables and limits for GOSAT-2. “–” means that no limit is applied.

Land			Water		
Variable	valid range		Variable	valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. optical depth s	-0.18	1.97 10 ⁻²	Scatt. optical depth s	8.82 10 ⁻³	2.97 10 ⁻²
Scatt. optical depth p	1.10 10 ⁻³	2.64 10 ⁻²	Scatt. optical depth p	7.66 10 ⁻³	5.41 10 ⁻²
Scatt. Ångström coeff. p	0.56	4.52	Pol. coeff. 1 win 6s	7.05 10 ⁻⁵	3.19 10 ⁻³
Surface roughness (m)	–	40.00	δD unc. (per mille)	–	76.39
Scatt. Ångström coeff. s unc.	0.12	1.00	Pol. coeff. 0 win 2s unc.	9.02 10 ⁻⁵	1.69 10 ⁻⁴
Pol. coeff. 1 win 1s	–	5.16 10 ⁻³	Pol. coeff. 2 win 6s unc.	4.32 10 ⁻⁵	1.58 10 ⁻⁴
Spectral shift win 5s unc.	–	3.71 10 ⁻⁴	Spectral squeeze win 2s	-3.44 10 ⁻³	1.48 10 ⁻³
Scatt. Ångström coeff. s	0.71	8.21	Pol. coeff. 3 win 2p	–	2.68 10 ⁻³
Pol. coeff. 3 win 2s	-1.72 10 ⁻³	2.48 10 ⁻³	Scatt. Ångström coeff. s unc.	7.11 10 ⁻²	1.00
Spectral squeeze win 3s	-5.96 10 ⁻⁴	1.00 10 ⁻³	Pol. coeff. 1 win 2s	6.70 10 ⁻⁴	8.15 10 ⁻³
Pol. coeff. 2 win 2s unc.	7.24 10 ⁻⁵	2.36 10 ⁻⁴	Pol. coeff. 3 win 4s unc.	2.14 10 ⁻⁵	4.89 10 ⁻⁴
Spectral squeeze win 3p	-5.67 10 ⁻⁴	1.76 10 ⁻³	Pol. coeff. 3 win 6s unc.	4.05 10 ⁻⁵	5.76 10 ⁻⁴



Table A7. XCH₄ filter variables and limits for GOSAT-2. “–” means that no limit is applied.

Variable	Land		Variable	Water	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. optical depth s	-0.18	1.91 10 ⁻²	Scatt. optical depth s	8.82 10 ⁻³	2.79 10 ⁻²
Scatt. optical depth p	-8.19 10 ⁻⁴	2.40 10 ⁻²	Scatt. optical depth p	3.36 10 ⁻³	3.59 10 ⁻²
Scatt. Ångström coeff. s unc.	0.14	1.00	Pol. coeff. 0 win 2s unc.	9.06 10 ⁻⁵	1.72 10 ⁻⁴
Surface roughness (m)	–	40.00	Pol. coeff. 1 win 6s	-4.19 10 ⁻⁵	3.85 10 ⁻³
χ ²	0.52	1.04	δD unc. (per mille)	8.03	56.34
Pol. coeff. 3 win 2p	–	5.35 10 ⁻³	Pol. coeff. 0 win 6p	3.34 10 ⁻²	0.36
Scatt. Ångström coeff. p	0.17	–	Pol. coeff. 3 win 2p	–	4.56 10 ⁻³
XCH ₄ unc. (ppm)	–	5.27 10 ⁻³	Spectral squeeze win 2s	-2.89 10 ⁻³	1.41 10 ⁻³
Pol. coeff. 1 win 4p	-1.56 10 ⁻²	-4.80 10 ⁻³	Scatt. Ångström coeff. s unc.	8.64 10 ⁻²	1.00
Pol. coeff. 1 win 1s	–	4.57 10 ⁻³	Pol. coeff. 1 win 2s	1.78 10 ⁻⁴	1.17 10 ⁻²
Scatt. Ångström coeff. s	0.29	8.21	Pol. coeff. 0 win 5s unc.	4.19 10 ⁻⁵	1.53 10 ⁻⁴
Pol. coeff. 3 win 2s	-1.72 10 ⁻³	3.41 10 ⁻³	Pol. coeff. 0 win 8p	4.88 10 ⁻²	0.28



Table A8. XCH₄ Proxy filter variables and limits for GOSAT-2. “–” means that no limit is applied.

Variable	Land		Variable	Water	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
XH ₂ O unc. (ppm)	2.84	13.70	XCO ₂ noise unc. (ppm)	–	1.84
χ^2	0.49	1.17	Pol. coeff. 0 win 5s unc.	–	$3.35 \cdot 10^{-4}$
XH ₂ O noise unc. (ppm)	–	16.64	Pol. coeff. 0 win 8p	$3.32 \cdot 10^{-2}$	–
Pol. coeff. 0 win 4p unc.	–	$1.03 \cdot 10^{-3}$	Pol. coeff. 0 win 4s unc.	–	$5.96 \cdot 10^{-4}$
Pol. coeff. 0 win 3s unc.	$5.97 \cdot 10^{-5}$	$3.55 \cdot 10^{-4}$	XH ₂ O noise unc. (ppm)	–	39.77
Pol. coeff. 0 win 4s unc.	$4.53 \cdot 10^{-5}$	$2.49 \cdot 10^{-4}$	Pol. coeff. 2 win 6s	$-3.26 \cdot 10^{-4}$	$3.78 \cdot 10^{-3}$
Spectral shift win 5s	$-6.64 \cdot 10^{-2}$	–	Scatt. Ångström coeff. s unc.	$3.33 \cdot 10^{-2}$	1.00
Spectral shift win 1p	-0.14	–	Pol. coeff. 1 win 2s	$-9.51 \cdot 10^{-4}$	$3.20 \cdot 10^{-2}$
Pol. coeff. 1 win 2s	$-5.63 \cdot 10^{-3}$	–			
Spectral squeeze win 8p	–	$1.12 \cdot 10^{-3}$			



Table A9. XH₂O filter variables and limits for GOSAT-2. “–” means that no limit is applied.

Land			Water		
Variable	valid range		Variable	valid range	
	min.	max.		min.	max.
δD unc. (per mille)	22.17	–	δD unc. (per mille)	16.47	–
Pol. coeff. 1 win 7p unc.	$1.18 \cdot 10^{-4}$	–	XH ₂ O noise unc. (ppm)	–	33.31
χ^2	0.78	–	Pol. coeff. 0 win 3s unc.	$8.84 \cdot 10^{-5}$	–
Pol. coeff. 0 win 4s unc.	$6.86 \cdot 10^{-5}$	–	Pol. coeff. 2 win 6p unc.	$4.66 \cdot 10^{-5}$	–
Surface roughness (m)	–	177.00	XCH ₄ smoothing unc. (ppm)	$7.52 \cdot 10^{-4}$	$3.70 \cdot 10^{-2}$
Pol. coeff. 0 win 2s unc.	$9.89 \cdot 10^{-5}$	–	Scatt. Ångström coeff. s	0.71	9.62



Table A10. δ D filter variables and limits for GOSAT-2. “–” means that no limit is applied.

Land			Water		
Variable	valid range		Variable	valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. optical depth p	$7.70 \cdot 10^{-3}$	–	Scatt. optical depth p	$1.60 \cdot 10^{-2}$	$7.64 \cdot 10^{-2}$
δ D unc. (per mille)	–	30.24	Scatt. optical depth s	$8.81 \cdot 10^{-3}$	$5.14 \cdot 10^{-2}$
XH ₂ O noise unc. (ppm)	6.58	52.74	δ D unc. (per mille)	–	27.86
XH ₂ O unc. (ppm)	7.12	53.71	XH ₂ O noise unc. (ppm)	6.78	125.86
SIF factor unc.	0.34	1.03	Pol. coeff. 3 win 2p	$-6.47 \cdot 10^{-3}$	$1.57 \cdot 10^{-3}$
Spectral squeeze win 2s unc.	$3.00 \cdot 10^{-4}$	$5.42 \cdot 10^{-4}$	Pol. coeff. 1 win 2s unc.	$8.97 \cdot 10^{-5}$	$3.38 \cdot 10^{-4}$
Pol. coeff. 1 win 6s	$-4.01 \cdot 10^{-3}$	$3.76 \cdot 10^{-3}$			



Table A11. XCO filter variables and limits for GOSAT-2. “–” means that no limit is applied.

Variable	Land		Variable	Water	
	valid range			valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. Ångström coeff. s unc.	$5.45 \cdot 10^{-2}$	–	XCO unc. (ppm)	–	$8.60 \cdot 10^{-3}$
Pol. coeff. 1 win 5s	$-1.27 \cdot 10^{-2}$	$2.19 \cdot 10^{-3}$	Pol. coeff. 1 win 2s	$7.57 \cdot 10^{-4}$	$3.50 \cdot 10^{-2}$
Pol. coeff. 2 win 5s	$-1.06 \cdot 10^{-3}$	–	XH ₂ O noise unc. (ppm)	–	22.72
Scatt. Ångström coeff. p unc.	$6.13 \cdot 10^{-2}$	–	Pol. coeff. 0 win 7s unc.	$5.40 \cdot 10^{-5}$	–
Pol. coeff. 1 win 2s	$-5.80 \cdot 10^{-3}$	–	Scatt. height s unc.	$4.99 \cdot 10^{-3}$	–
XCH ₄ smoothing unc. (ppm)	$7.99 \cdot 10^{-4}$	–	Pol. coeff. 2 win 7s unc.	$1.41 \cdot 10^{-4}$	–
XCO unc. (ppm)	–	$9.62 \cdot 10^{-3}$	Scatt. Ångström coeff. s unc.	$3.76 \cdot 10^{-2}$	–



Table A12. XN₂O filter variables and limits for GOSAT-2. “–” means that no limit is applied.

Land			Water		
Variable	valid range		Variable	valid range	
	min.	max.		min.	max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
Scatt. optical depth s	–	1.74 10 ⁻²	Scatt. optical depth s	–	2.43 10 ⁻²
Scatt. optical depth p	–	0.11	Scatt. optical depth p	–	0.11
Spectral squeeze win 6s unc.	–	1.74 10 ⁻⁴	Pol. coeff. 0 win 4s	0.11	–
Spectral squeeze win 7s unc.	–	4.24 10 ⁻⁴	Spectral squeeze win 3p unc.	–	9.81 10 ⁻⁴
Spectral shift win 7p unc.	–	5.63 10 ⁻⁴	Spectral shift win 2s unc.	–	6.77 10 ⁻⁴
Spectral squeeze win 7p unc.	–	4.16 10 ⁻⁴	Pol. coeff. 0 win 8s	3.71 10 ⁻²	–
Spectral shift win 8s unc.	3.46 10 ⁻⁴	4.68 10 ⁻⁴	N ₂ O unc. (ppm)	4.34 10 ⁻³	7.88 10 ⁻³
Pol. coeff. 1 win 1s	–	4.57 10 ⁻³	XCO ₂ unc. (ppm)	–	4.23
N ₂ O unc. (ppm)	3.90 10 ⁻³	9.05 10 ⁻³	Pol. coeff. 0 win 6s	0.11	–
Scatt. Ångström coeff. s unc.	9.32 10 ⁻²	–	δD unc. (per mille)	–	55.78
Spectral shift win 7s unc.	–	7.11 10 ⁻⁴	Pol. coeff. 2 win 2p unc.	1.08 10 ⁻⁴	3.24 10 ⁻⁴
XCO unc. (ppm)	2.03 10 ⁻³	6.25 10 ⁻³	Pol. coeff. 1 win 8s	2.15 10 ⁻³	–