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

by S. Noël et al.

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Authors' Response

Reply to referee 1

We thank the referee for the very detailed and constructive comments. Since the comments were given in the PDF file of the paper, we have added our response also to this file, see attachment.

Reply to referee 2

We thank the referee for the review and the comments. They will be considered in the revised version of the paper. In the following, the original reviewer comments are given in *italics*, our answer in normal font.

This paper presents a new retrieval (FOCAL 3.0) for XCO2, XCH4, XH2O, XCO, HDO, and XN2O from GOSAT and GOSAT-2. It is exciting to see retrievals from GOSAT-2. The retrievals are validated following standard protocols. I was very interested by the scatter and temporal bias metrics relative to TCCON – they are not usually shown but I found them very instructive. I recommend publication in AMT but suggest that the authors consider the following comments:

1. *The Introduction advertises that comparisons with previous satellite products will be shown but I could not find these comparisons in the text.*

   The TCCON comparisons include also comparisons with other GOSAT satellite products using the same reference stations. This allows a direct comparison of results, see Tab. 6 and corresponding figures. We already address this in the related text, but we will clarify this in the revised version.

2. *Equation (1) suggests that methane must be retrieved by the full-physics algorithm in order to derive a proxy estimate but that would erase much of the benefit of the proxy method in enabling successful retrievals when the full-physics method can't.*

   Indeed, the XCH4 proxy product is derived by using as input the results from the XCH4 full-physics product. However, we use different (more relaxed) post-processing filters for the proxy product. This results in more valid data than all other GOSAT proxy products (see Fig. 1) with good quality (see TCCON comparisons), and it does not require e.g. a dedicated non-scattering retrieval. Retrieving all products with a single retrieval run is actually a main benefit of our method. We will emphasise the latter a bit more in the revised version.

3. *Gradients in Figures 2 and 3 are so washed out as to make the Figures useless.* We will adapt the colour scale of the plots to emphasise the gradients where required. Note that this is somewhat limited as we deliberately use a conceptionally uniform colour table.

4. *Line 390: 'the data sets...are available from the authors'. That's OK at the submission stage but won't do at the publication stage. The data sets should be publicly posted.* We will clarify this with AMT if required. For other recent publications we had no problem with this.

Reply to referee 3

We thank the referee for the review and the comments. They will be considered in the revised version of the paper. In the following, the original reviewer comments are given in *italics*, our answer in normal font.

The updated FOCAL retrieval (v3) is presented in this paper. It can process GOSAT and GOSAT-2 data. It has improved capabilities, mostly bigger spatial coverage than its predecesors, new molecular species measured and new processing. It can measure CO2, CH4, H2O, HDO, CO and N2O.
The paper is well written and well presented, and, as such, deserves publsihing. Some minor comments would improve the readability of the paper.
Unfortunately, it has been written in a manner that serves solely as a reference, since most of the content are references to previous papers. It is therefore very dull to read and has very little "information" appart from some uncertainty figures, sepcially for someone outside of the field . Since the style of the paper cannot be modified substantitally because this would mean a huge effort, I suggest to include the following additions:

1. *It should be stated, in the abstract, the beggining and in section "3.2 Processing" whether the uncertainties of the retrievals are determined. A great emphasis is placed on the amounts derived, but very little in the uncertainties. Are the uncertainties for each individual "pixel" determined? Or can a global uncertainty figure be derived?*

   The uncertainties are determined for each ground pixel. We will clarify this in the revised version as requested.

2. *In line with the previous statement, include a sentence or two describing, in general, the algorithm used for pre-processing, processing and post-processing. Is it something similar to a linear regression? Non-linear regression? Machine learning? Optimal estimation? Please include some phrases such that the reader does not need to read one or two other papers to understand in general terms how the retrieval works.*

   The retrieval is based on optimal estimation. We will include a short description in the revised version.

3. *In the conclusion, for a reader outside from this field, it is not known whether these retrievals will make a difference in the community or not. Do they satisfy the requirements to geographycally locate the sources and sinks of CO2? CH4? Do they satisfy some requirements that can be useful to the communitty? Can they be assimilated in an AC numerical model? If not, which requirements would be needed in future instruments? In summary, a paragraph to show that this work is useful for humanity and not just for the machines that are being fed the numbers.*

   We will add some information about then relevance of the results in the conclusions.

Reply to referee 4

We thank the referee for the review and the comments. They will be considered in the revised version of the paper. In the following, the original reviewer comments are given in *italics*, our answer in normal font.

This paper describes the new v3.0 FOCAL retrievals for GOSAT and GOSAT-2, used to retrieve XCO2, XCH4, XCO, XNO2, XH2O, and the relative ratio of semi-heavy water to water vapour. The paper describes the methods used in the retrievals and validates the new dataset against the TCCON network. Overall, the paper clearly describes the retrieval methods and demonstrates the value of the new data products. Therefore, I recommend publication, with several minor revisions based on the comments below.

Specific comments

1. *Title: Should the title list the species being retrieved?*

   We think listing all species in the title would make it too long. We will actually shorten the title as suggested by Referee #1.

2. *Abstract: Are the new FOCAL v3.0 datasets publicly available?*

   The FOCAL data are available by request from the authors as stated later in the paper.

3. *Line 10: I found this paragraph a bit difficult to follow. For lines 10-11, do you mean something like this? "For XCO2, the new FOCAL retrieval (v3.0) significantly increases the number of valid XCO2 data compared with the previous FOCAL retrieval version (v1) by 50% for GOSAT and about a factor of two for GOSAT-2." Are "All FOCAL data products" in line 11 referring to all v3.0 data products?*

   We will update the text accordingly and clarify that we refer to v3 products.

4. *Line 165: For the filtering procedure - how do you ensure that real variability isn't accidently filtered out from the dataset?*

   Real variability (e.g. local sources) are not filtered out as long as there are no correlations between the filter variable and e.g. a local XCO2 enhancement. This is why we use a very restricted set of possible variables and a large test data set (one full year). This will be explained in the revised version.

5. *Line 216: Could you add a brief definition of the full physics vs proxy datasets for CH4 and explain why there are more data for the proxy products? Are the full physics and proxy comparable or do they have different applications/uncertainties?*

   The proxy data are less sensitive to light path / scattering effects which allows for a relaxed filtering in post-processing and therefore more data. The error of the XCH4 proxy product is in fact larger than for the full physics product, because it includes also the error of the retrieved XCO2. We will mention this in the revised version.

6. *Line 252: Add a brief description of the CO2 timeseries to the text since this is also shown in the figure? Is the timeseries qualitatively in line with other versions of the CO2 retrieval? Other monitoring?*

   We will add this.

7. *Line 263: Is there also no temporal trend in delta_D? Is it expected that year-to-year variations for delta_D be larger?*

   From visual inspection of the time series it seems that GOSAT delta_D is slightly decreasing. We cannot tell if this is significant or not without a detailed trend analysis, which would be a subject of its own and beyond the scope of this paper. Note that trends may also be effected by the varying

sampling of the data over time (see Fig. 1). Therefore we do not discuss a possible delta_D trend here.

Year-to-year variations are also affected by sampling. The prominent peaks in July 2012 in the southern hemisphere and in December 2018 in the northern hemisphere are due to very few data in these regions in these months. We will explain this in the paper.

8. *Line 287: Please add a bit more detail about the comparison quantities being calculated. Perhaps including formulae would be helpful. For example, how is the seasonal variation of the difference at each station being calculated?*

   We use a well established validation method which we also used in the v1 paper. The seasonal bias is derived from a trend fit as mentioned later in the text. A detailed description of the method (incl. formulas) is given in:

   Reuter, M. and Hilker, M.: End-to-End ECV Uncertainty Budget Version 3 (E3UBv3) for the FO-CAL XCO2 OCO-2 Data Product CO2_OC2_FOCA (v10), Tech. Rep. version 3, 6 Feb 2022, ESA Climate Change Initiative "Plus"(CCI+), `https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/CRDP7/E3UBv3_GHG-CCI_CO2_OC2_FOCA_v10.pdf`.

   We will replace the reference to Reuter et al. (2019b) by this reference in the text.

9. *Figure 1: This figure takes a bit of effort to read. Is there a reason that the full timeseries is shown instead of, e.g., a summary of the count during the measurement period with all available datasets? If so, describe the timeseries more in the text. Perhaps it would be easier to read if colours were used consistently across figure panels and if the FOCAL data product was somehow distinguished from the other products (e.g., with a distinct colour choice, cross-hatching or something else?). In panel (d), could the FOCAL v1.0 and focal v3.0 XCO2 be put next to each other so that they can be more easily compared?*

   As can be seen in this figure, the number of data products varies with time and therefore also the sampling of data. We already discussed this in the previous (v1) paper, but will add some info on this in the revised version.

   As suggested by referee #1 we will split the figure into two parts:

   - Subfigures (a) and (b) for GOSAT XCO2 and XCH4 from all algorithms.
   - Subfigures (c) and (d) for all other (FOCAL) products.

   We will adjust colours to make them more consistent within each of these plots and also mark data from different retrieval teams with different hatches. FOCAL v1 and v3 XCO2 will be put next to each other in the last sub-figure.

10. *Figures 6-10 are barely described in the text. Can these be moved into an appendix or the supplementary material? Also, please make font sizes bigger. Tables: There are a lot of tables included in the paper. Some of these are not referenced from anywhere in the text (Table 2, 4, 5). Are all tables needed in the main body of the text - if so add descriptive text. (Otherwise, could move to appendix or supplement)*

    Figures 6-10 include information on individual TCCON stations, therefore we prefer to keep them in the main part.

    We will modify / split / combine these figures also following the comments of the other referees. Increasing font sizes is however somewhat limited as figure width is limited by AMT and the text has to fit into the layout of the plots (which is difficult especially if many products are shown as for XCH4). We will try our best on this.

Technical comments

1. *Line 266: Rephrase so that it is clear what XCO is similar to. E.g., "Across different latitudes, GOSAT-2 XCO shows similar values and seasonal variations, except in the southern hemisphere..."*

Will be changed.

List of changes

Changes according to the comments mentioned above have been made in the revised manuscript. Especially, some figures have been removed or combined and some have been added. Therefore, figure numbering has changed. The changes are marked in a corresponding version of the revised manuscript provided separately.

Attachment:

- Commented manuscript with answers to referee #1 (may require Acrobat reader or similar tool to correctly see answers).

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 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$_2$O) 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$_2$O) for which we also show first results. We also present an update on XCO$_2$ from both instruments.

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$_2$O product. Global XN$_2$O 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$_2$O product compares well with TCCON. Its station-to-station variability is lower than 2 ppb, which is about the magnitude of the typical N$_2$O variations close to the surface. However, both GOSAT-2 and TCCON measurements show that the seasonal variations in the total column average XN$_2$O are in the order of 8 ppb peak-to-peak, which can be easily resolved by the GOSAT-2 FOCAL data.

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 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 optimised for, a single product. However, the derivation of a specific product usually requires the consideration of various additional atmospheric constituents and processes.

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 retrievaL) 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 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

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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://prdct. 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.

input spectra, we use calibrated GOSAT and GOSAT-2 L1B radiances of the three NIR/SWIR bands at around 0.76, 1.6 and $2.0\,\mu m$. 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 XCO_2 and XCH_4. These are now derived using a Simple cLImatological Model for atmospheric CO_2 and CH_4, 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 XCO_2 and XCH_4. 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 XCO_2 and XCH_4, namely the ACOS v9r XCO_2 product from NASA (Taylor et al., 2022); the full physics and proxy products from the University of Leicester (UoL XCO_2 and XCH_4 FP v7.3, UoL XCH_4 proxy v9.0; Cogan et al., 2012); the full physics and proxy products from SRON (RemoTeC FP XCO_2 and XCH_4 v2.3.8, RemoTeC XCH_4 proxy product v2.3.9; Butz et al., 2011); and the operational bias-corrected GOSAT XCO_2 and XCH_4 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 XCO_2 and XCH_4.

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 retrievaL (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 H_2O 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 XN_2O window where a degree of 4 is used.

All quantities in the state vector are retrieved simultaneously. For CO_2, CH_4 and H_2O we derive profiles on 5 layers which are then converted to total column average D, XCO and XN_2O are derived via scaling factors. The XCH_4 proxy product is derived after the retrieval from these full physics products (see below). In the case of GOSAT-2, all scattering parameters as 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
115 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 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.

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3. Bias correction (for CO_2 and CH_4 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 XCH_4 proxy product is computed during post-processing from:

$$XCH_4^{proxy} = XCH_4^{retrieved} \frac{XCO_2^{apriori}}{XCO_2^{retrieved}} \tag{1}$$

This means we normalise the retrieved full physics XCH_4 by the retrieved full physics XCO_2 (both without bias correction) and use as reference the a priori XCO_2. Note that this is different to e.g. the SRON XCH_4 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 XCH_4 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. XCO_2, methane and water vapour products). For the ~~others,~~ i.e. XCO and XN_2O, 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 XN_2O. This is to avoid that e.g. a valid ~~XCO_2 measurement is filtered out due to a bad~~

155 ~~XN_2O 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 XCO_2. 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.

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

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 $15° \times 15°$ 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 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.

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 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 CO_2 gradient at the surface is also not used anymore, as this might result in filtering out scenes with too high CO_2 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 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 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 XCO_2 and the XCH_4 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 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" XCO_2 and XCH_4. 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 XCO_2 and ± 10 ppb for XCH_4 with corresponding TCCON data. The "best" parameters have been chosen from essentially the same list of candidate 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.

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 XCO_2 and XCH_4 uncertainties via a linear function he 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 use data from the SLIMCO2/SLIMCH4 reference database as "true" values.

4   Results

All GOSAT and GOSAT-2 a until the end of 2020 have been essed. Fig. ows 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 XCO_2 products are also shown. Fig. 1a compares the number of yearly GOSAT-FOCAL XCO_2 data with other available GOSAT data products from SRON, the University of Leicester (UoL), NIES and NASA (ACOS product similar comparison is shown in Fig. 1b for XCH_4 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 XCO_2 and methane results exceeds those of all other GOSAT data sets.

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

For each of the different data products an example map comprising a mean for April 2019, gridded to $5° \times 5°$, 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 XCO_2 look very similar for GOSAT and GOSAT-2. GOSAT-2 data show in general fewer gaps over the oceans, but with smaller latitudinal coverage. latter is due to the currently applied RSR filtering for GOSAT-2, which especially removes data over water surfaces. Note that over the year the spatial range of valid data varies according to illumination conditions.

8

The XCO_2 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.

Water vapour (XH_2O) 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 H_2O. The observed spatial distribution of δD is in line with the maps shown in Frankenberg et al. (2013).

For GOSAT-2 there are also data for carbon monoxide (XCO) and XN_2O. 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 XN_2O product shows an overall decrease of the background XN_2O from the tropics to higher latitudes in the order of 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 XN_2O 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 XN_2O gradient can, in principle, be explained by the variation of the tropopause height. As most of the XN_2O is contained (and well mixed) in the troposphere, the total column average is larger in the tropics (where the tropopause is high) than at higher latitudes. We also see increased XN_2O 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 southern latitudes with usually more variability in the north.

The methane full physics and proxy products show a similar temporal variation with increasing XCH_4 (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 XCH_4 full physics and the proxy products can be explained by the broader spatial coverage of the proxy product.

For water vapour (XH_2O), 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 2021.

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 large for δD.

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 XN_2O 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 XN_2O, 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 XN_2O, for which other spatial variations are low. In the tropics, the XN_2O data are always high, and the variations are much smaller. In fact, we see a slight increase in XN_2O of about 1 ppb per year, 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 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.

For XCO_2 and XCH_4 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.

– 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 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 XCO_2). 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 XCH_4 proxy products, as well as the XH_2O and XCO products, have the largest number of collocations because of the relaxed filtering.

4.3.1 XCO_2 results

For GOSAT FOCAL v3.0 the XCO_2 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 XCO_2, 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   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).

GOSAT-2 XCO_2 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 XCH$_4$ results

The full physics XCH$_4$ 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 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 XCH$_4$ product and 6.2 ppb for the proxy.

The mean scatter of the GOSAT and GOSAT-2 FOCAL XCH$_4$ product is around 12 ppb, which is slightly lower than for 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 XCH$_4$ 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 XH$_2$O results

Since water vapour is highly variable, the comparison results depend strongly on the involved TCCON stations. Because of the less strict filter criteria for XH$_2$O 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 XH$_2$O. 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 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 δD results

For δD 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 δD data, so all numbers given here should be treated with caution. 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 XN$_2$O 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. 10), 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 XN$_2$O results

The FOCAL XN$_2$O is a new data product that is so far not available from other GOSAT-2 retrievals. For XN$_2$O 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. 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 XN$_2$O are similar to the expected local XN$_2$O variability of a few ppb (see e.g. Garcia 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 XCO. 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 XCO$_2$ 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 XH$_2$O 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 XN$_2$O 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 CO_2 or CH_4" SLIMCO2 or SLIMCH4 has been developed to provide estimates of dry-air mole fraction profiles and column averages of atmospheric CO_2 or CH_4 with reasonable accuracy at minimum computational costs. A key application of SLIMCO2 or SLIMCH4 is to compute CO_2 or CH_4 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 CO_2 mole fraction data of NOAA's CarbonTracker model version CT2019B Jacobson et al. (2020). It has the same $3° \times 2°$ 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 CH_4 mole fraction data (Bergamaschi et al., 2013) with a spatial resolution of $6° \times 4°$. 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 CO_2.

First, we computed the global mean XGAS (XCO_2 or XCH_4) 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 CO_2 and 1984-2020 for CH_4, 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 CO_2 and CH_4 computed from global

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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 CO_2 or CH_4 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 XCO_2 and XCH_4 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 CO_2, 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 XCO_2 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 CH_4, 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 CO_2 biases with a station-to-station standard deviation of 0.57 ppm and an average scatter of 1.14 ppm (Fig. A5a). For CH_4, 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 XCO_2, 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.

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23
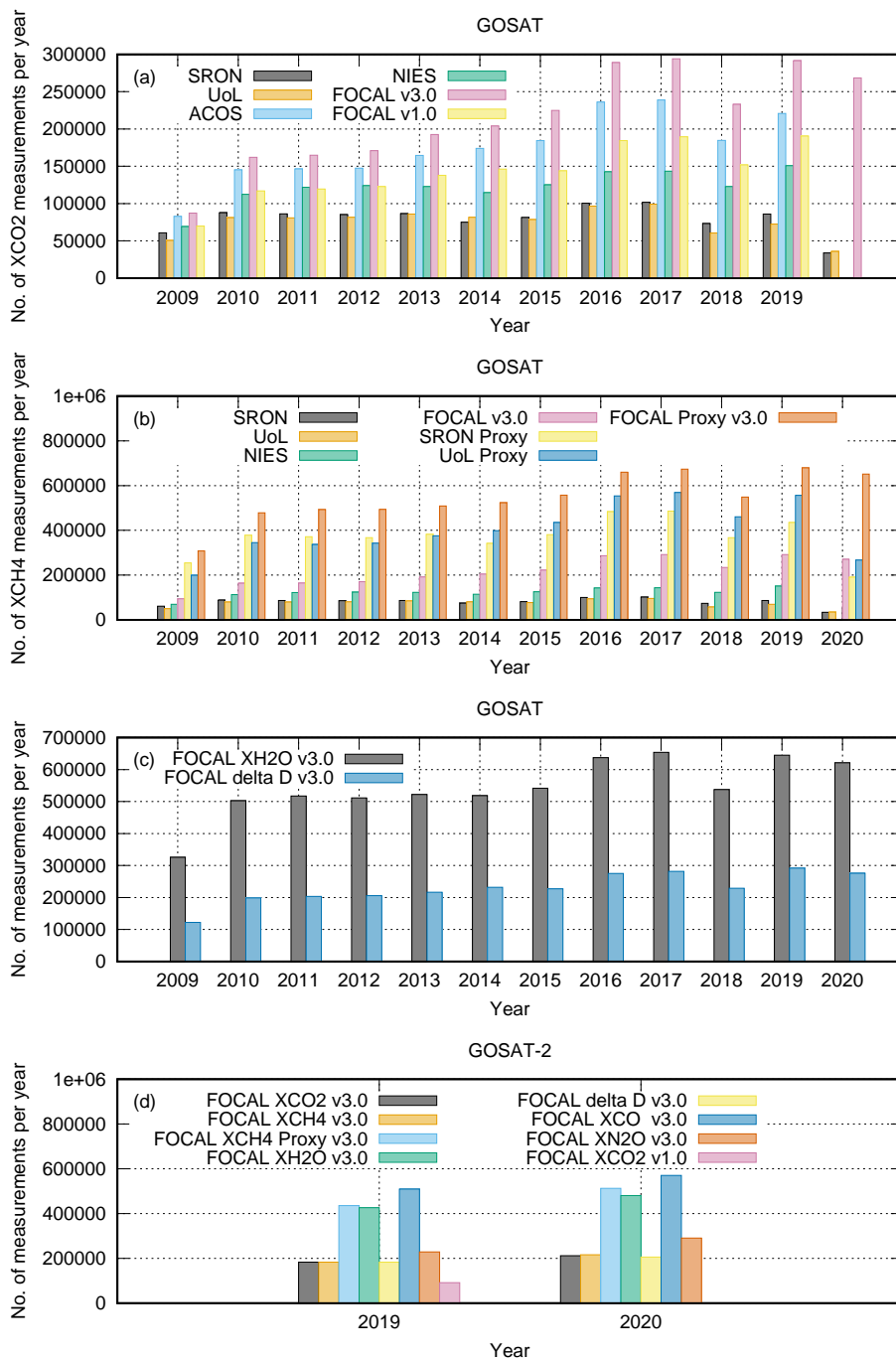
Figure 1. Number of GOSAT and GOSAT-2 data for different products as function of time (see Tab. 6 for details on version numbers). (a) GOSAT XCO_2. (b) GOSAT XCH_4. (c) GOSAT FOCAL XH_2O and δD. (d) GOSAT-2 FOCAL products
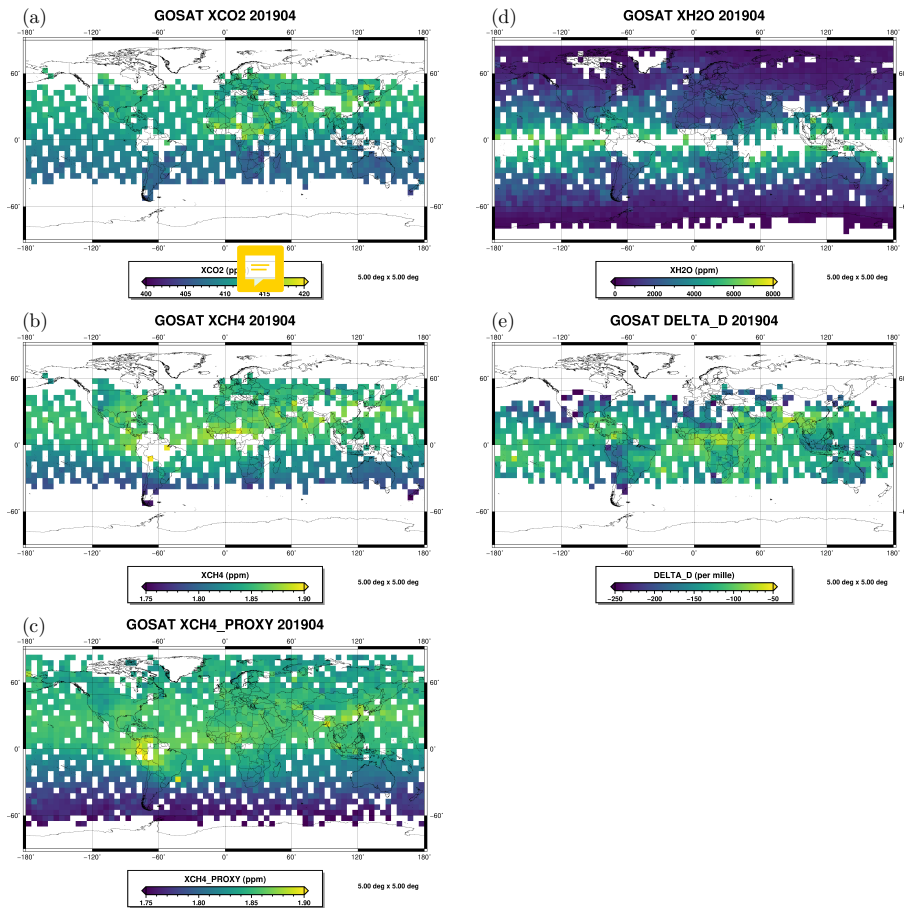
Figure 2. Maps of gridded GOSAT data for April 2019: (a) XCO_2. (b) XCH_4 full physics product. (c) XCH_4 proxy product. (d) XH_2O. (e) δD.
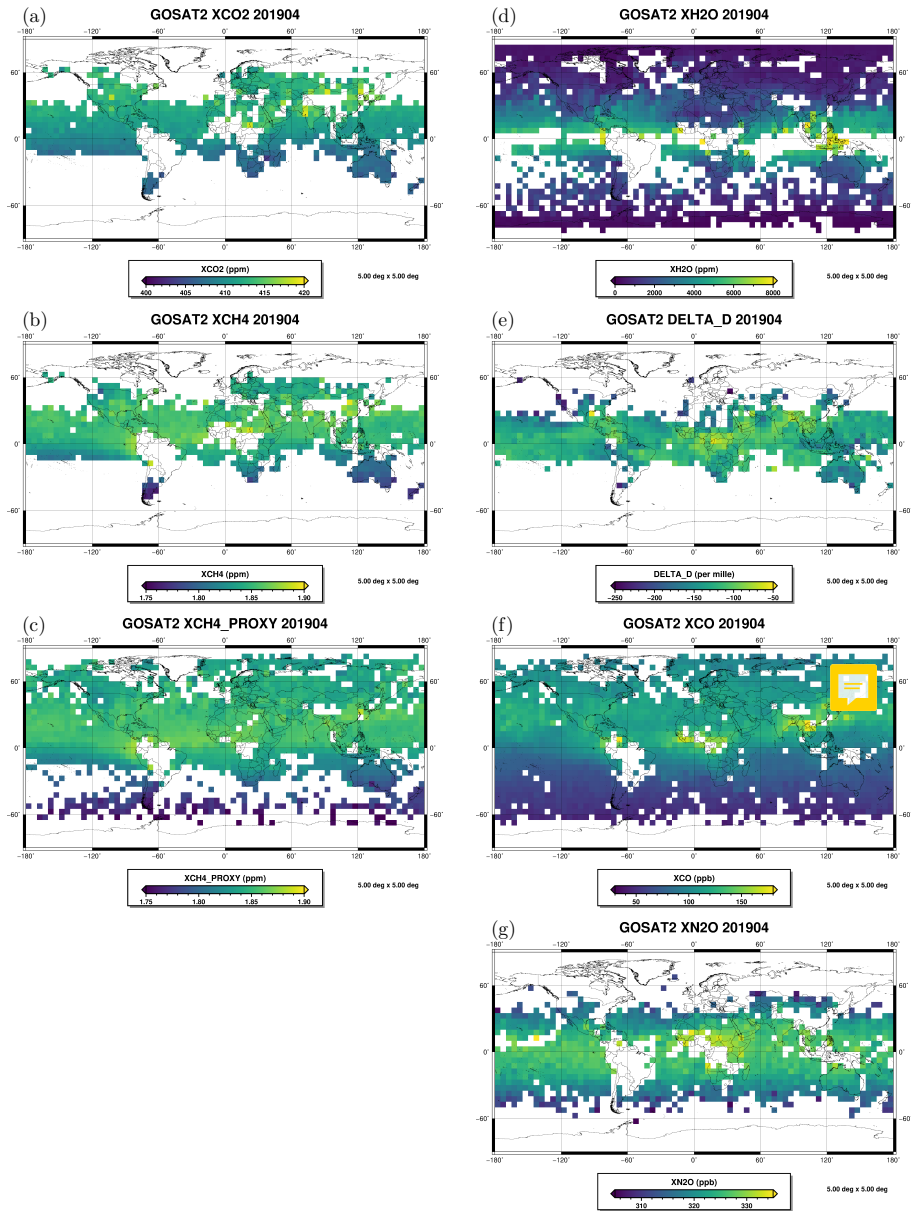
Figure 3. Maps of gridded GOSAT-2 data for April 2019: (a) XCO_2. (b) XCH_4 full physics product. (c) XCH_4 proxy product. (d) XH_2O. (e) δD. (f) XCO. (g) XN_2O.
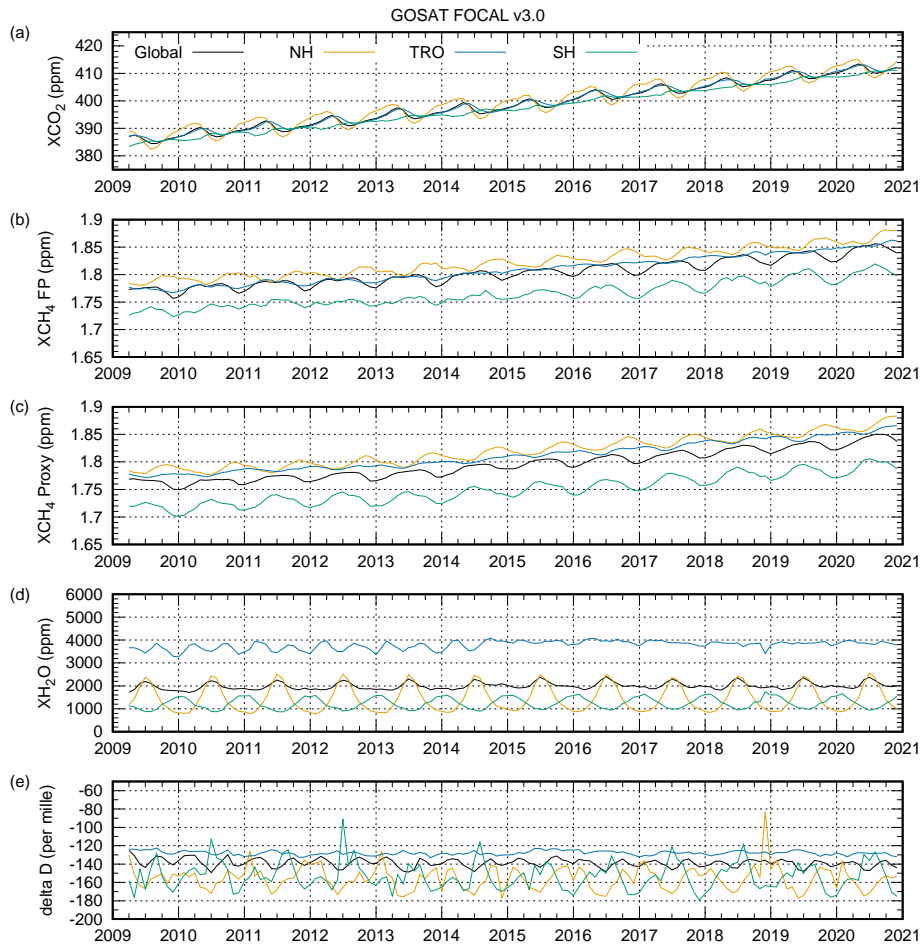
Figure 4. GOSAT time series. NH = Northern hemisphere ($> 25°$N). TRO = Tropics ($25°$S – $25°$N). SH = Southern hemisphere ($< 25°$S). (a) XCO_2. (b) XCH_4 full physics product. (c) XCH_4 proxy product. (d) XH_2O. (e) δD.

Figure GOSAT-2 time series. NH = Northern hemisphere ($> 25°$N). TRO = Tropics ($25°$S – $25°$N). SH = Southern hemisphere ($< 25°$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.

(a) XCO$_2$

ACOS v9r
UoL v7.3
SRON v2.3.8
NIES v2.9xbc
FOCAL v3.0

Bias [ppm]   Scatter [ppm]

Sodankylä
East Trout Lake
Bialystok
Bremen
Karlsruhe
Paris
Orleans
Garmisch–Partenkirchen
Park Falls
Rikubetsu
Indianapolis
Four Corners
Lamont
Tsukuba_tk
Edwards
Pasadena_jf
Pasadena_ci
Saga
Hefei
Burgos
Ascension Island
Darwin
Reunion Island
Wollongong

Overall   0.44 / 0.53 / 0.59 / 0.54 / 0.51   1.66 / 1.83 / 2.12 / 2.02 / 2.19

(b) XCH$_4$

UoL v7.3
SRON v2.3.8
NIES v2.9xbc
FOCAL v3.0
UoL pr_v9.0
SRON pr_v2.3.9
FOCAL v3.0 Proxy

Bias [ppb]   Scatter [ppb]

Sodankylä
East Trout Lake
Bialystok
Bremen
Karlsruhe
Paris
Orleans
Garmisch–Partenkirchen
Park Falls
Rikubetsu
Indianapolis
Four Corners
Lamont
Tsukuba_tk
Edwards
Pasadena_jf
Pasadena_ci
Saga
Hefei
Burgos
Ascension Island
Darwin
Reunion Island
Wollongong

Overall   5.2 / 5.0 / 3.6 / 4.6 / 3.4 / 6.1 / 4.3   13.3/13.5/13.4/14.0/12.6/12.8/12.4

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$_2$O. (d) δD.

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(a) XH$_2$O

Bias [ppm]
Scatter [ppm]

FOCAL v3.0 —

Eureka
Ny Alesund
Sodankylä
East Trout Lake
Bialystok
Bremen
Karlsruhe
Paris
Orleans
Garmisch–Partenkirchen
Park Falls
Rikubetsu
Lamont
Anmeyondo
Tsukuba_tk
Edwards
Pasadena_jf
Pasadena_ci
Saga
Darwin
Wollongong
Lauder_ll
Lauder_lh
Lauder_lr

Overall   116.1   304.0

(b) δD

Bias [per mille]
Scatter [per mille]

FOCAL v3.0 —

Sodankylä
East Trout Lake
Bialystok
Bremen
Karlsruhe
Paris
Orleans
Garmisch–Partenkirchen
Park Falls
Rikubetsu
Lamont
Anmeyondo
Tsukuba_tk
Edwards
Pasadena_jf
Pasadena_ci
Saga
Hefei
Burgos
Manaus
Ascension Island
Darwin
Reunion Island
Wollongong

Overall   8.6   32.9

Figure 7. As Figure 6, but for: (a) XH$_2$O. (b) δD.

30
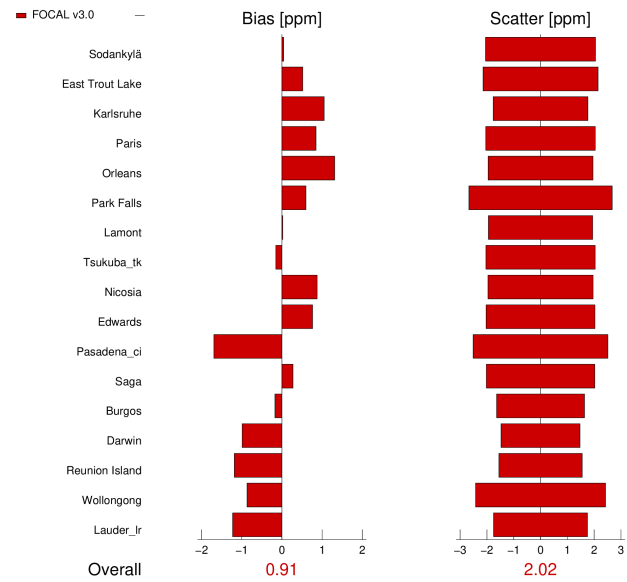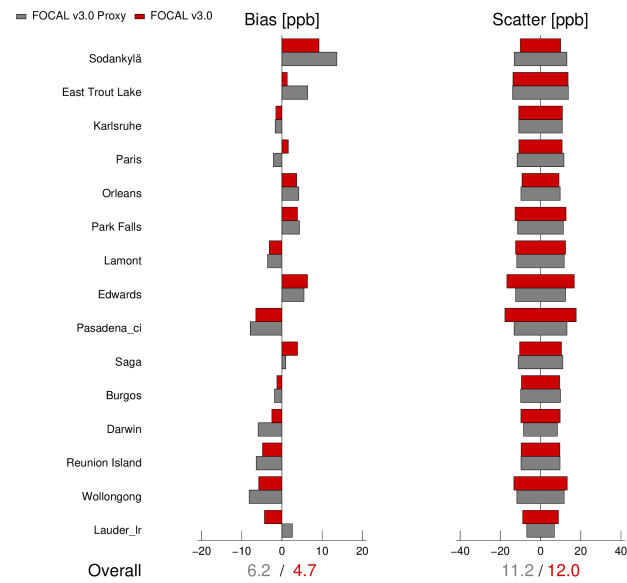
Figure 8. Overview of comparison results between GOSAT-2 FOCAL products and TCCON data: Scatter and bias for different TCCON stations. Note that the mean station bias has been subtracted to better illustrate the local station differences. (a) XCO_2. (b) XCH_4 (full physics and proxy products).

(a) XH_2O
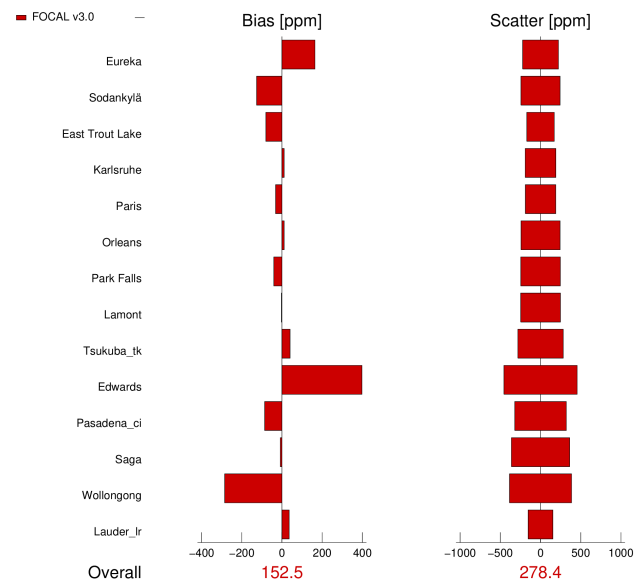
(b) δD
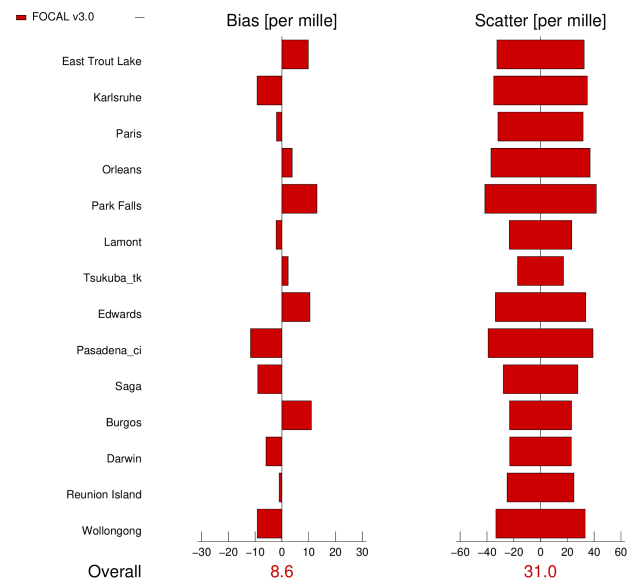
Figure 9. As Fig. 8, but for: (a) XH_2O. (b) δD.
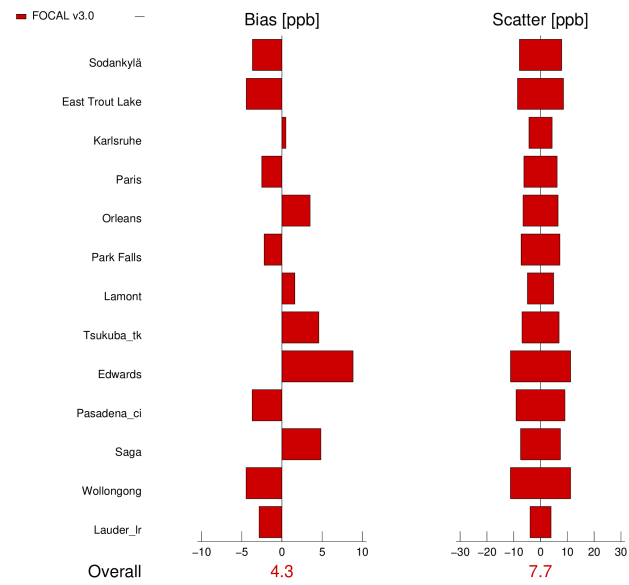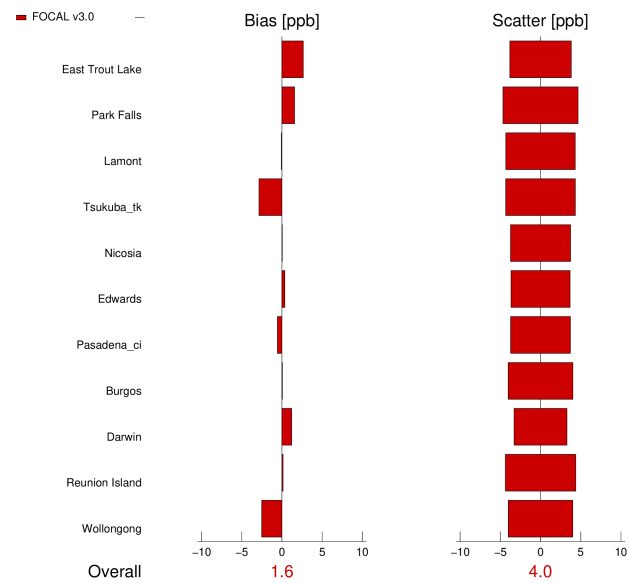
Figure 10. As Fig. 8, but for: (a) XCO. (b) XN$_2$O.
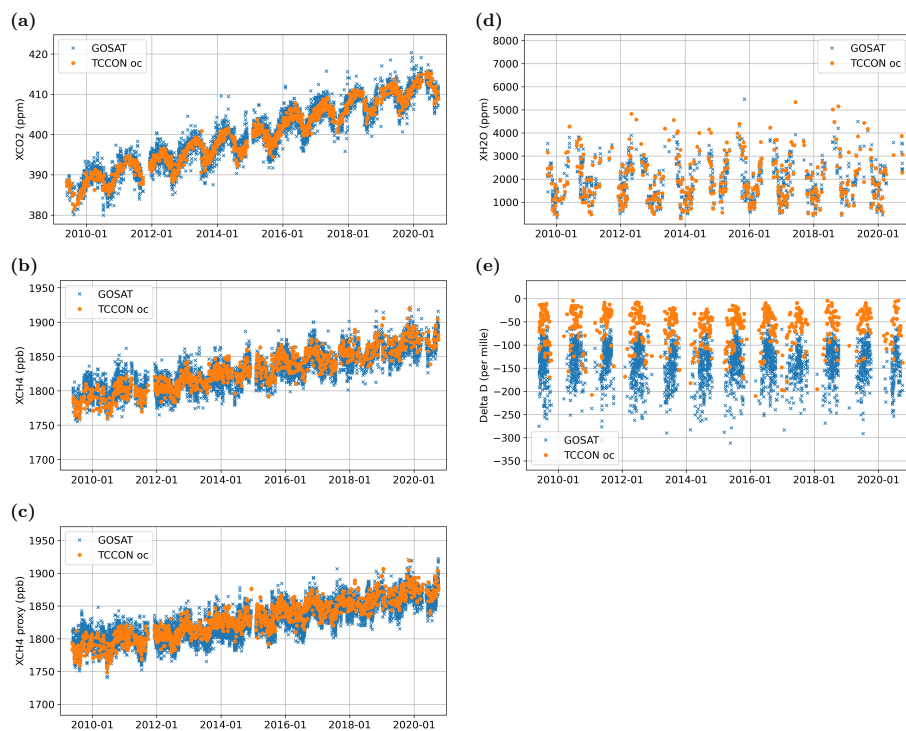
Figure 11. Example time series of TCCON and GOSAT FOCAL data at Lamont (station code oc). (a) XCO_2. (b) XCH_4 full physics product. (c) XCH_4 proxy product. (d) XH_2O. (e) δD.
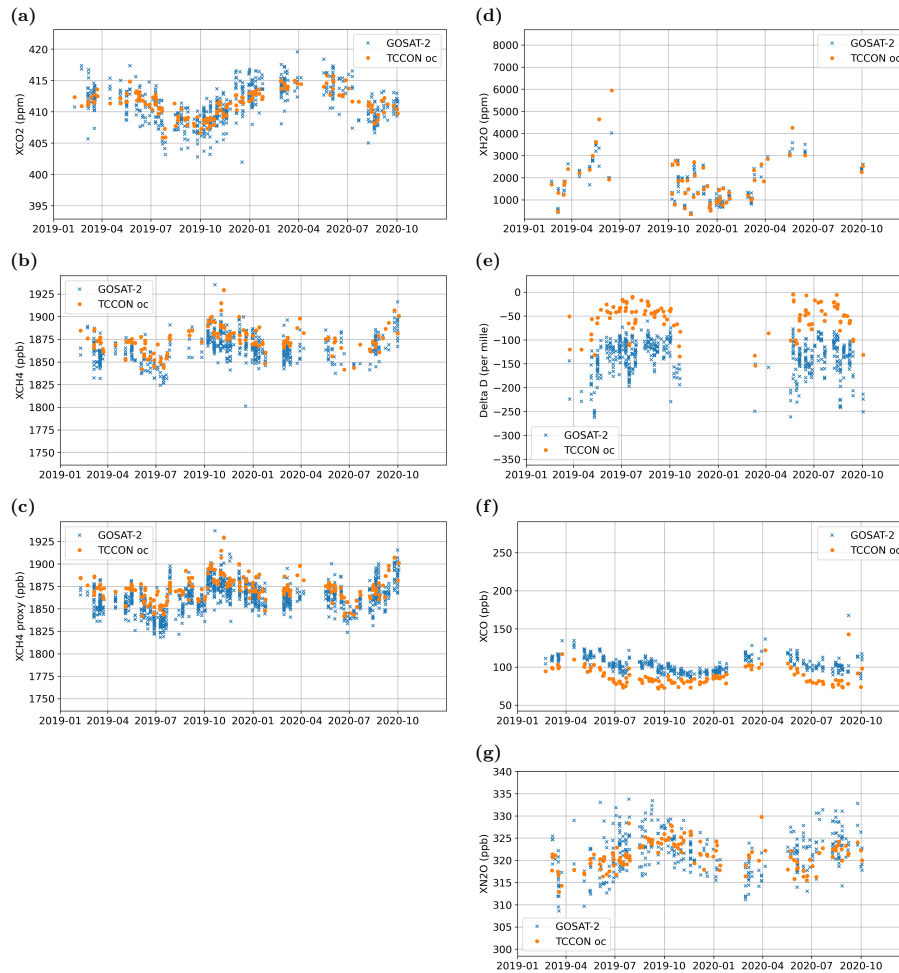
Figure 12 Example time series of TCCON and GOSAT-2 FOCAL data at Lamont (station code oc). (a) XCO_2. (b) XCH_4 full physics product. (c) XCH_4 proxy product. (d) XH_2O. (e) δD. (f) XCO. (g) XN_2O.

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_2O^a, O_3^b
2	O_2	12930 – 13170	O_2^a, H_2O^a, O_3^b
3	HDO	6337 – 6410	CO_2, H_2O, HDO, CH_4
4	CO_2	6161 – 6297	CO_2^a, H_2O, HDO, CH_4
5	CH_4	5945 – 6135	CO_2, H_2O, HDO, CH_4
6	CO_2	4801 – 4907	CO_2^a, H_2O, HDO
7	N_2O	4364 – 4449	N_2O, H_2O, HDO, CH_4
8	CO	4228 – 4328	CO , H_2O, 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_2O 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_2O 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_2O 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_2O	–	–	30%
δD	75°	40%	50%
XN_2O	75°	40%	50%
XCO	75°	–	20%
Water			
XCO_2	75°	40%	40%
XCH_4	75°	40%	40%
XCH_4 Proxy	75°	–	20%
XH2O	–	–	30%
δD	75°	40%	40%
XN_2O	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 Prox	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 Prox	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_2O (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_2O (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_2O (ppb)	11	3151	0.63	1.61	4.02	1.56

[a] XCH_4 Proxy validated together with full physics product, i.e. for same subset of TCCON stations
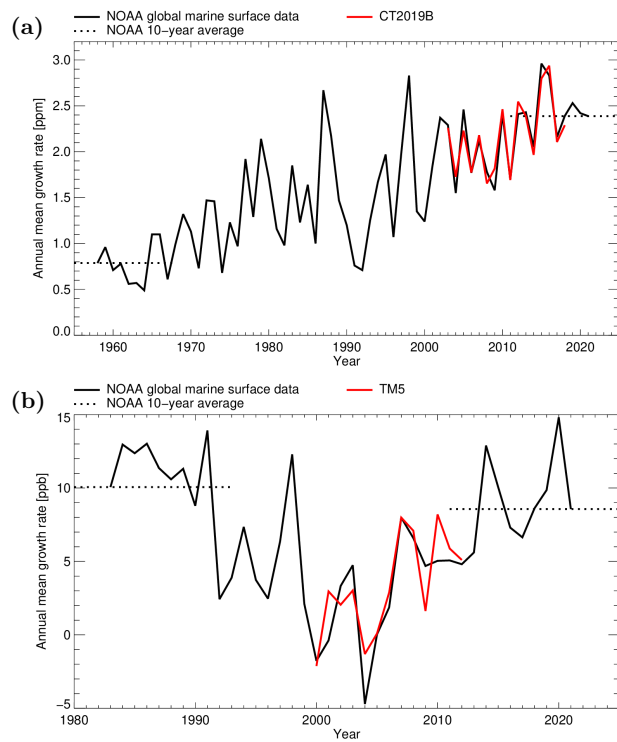
Figure A1. Global growth rates for CO_2 (a) and CH_4 (b).
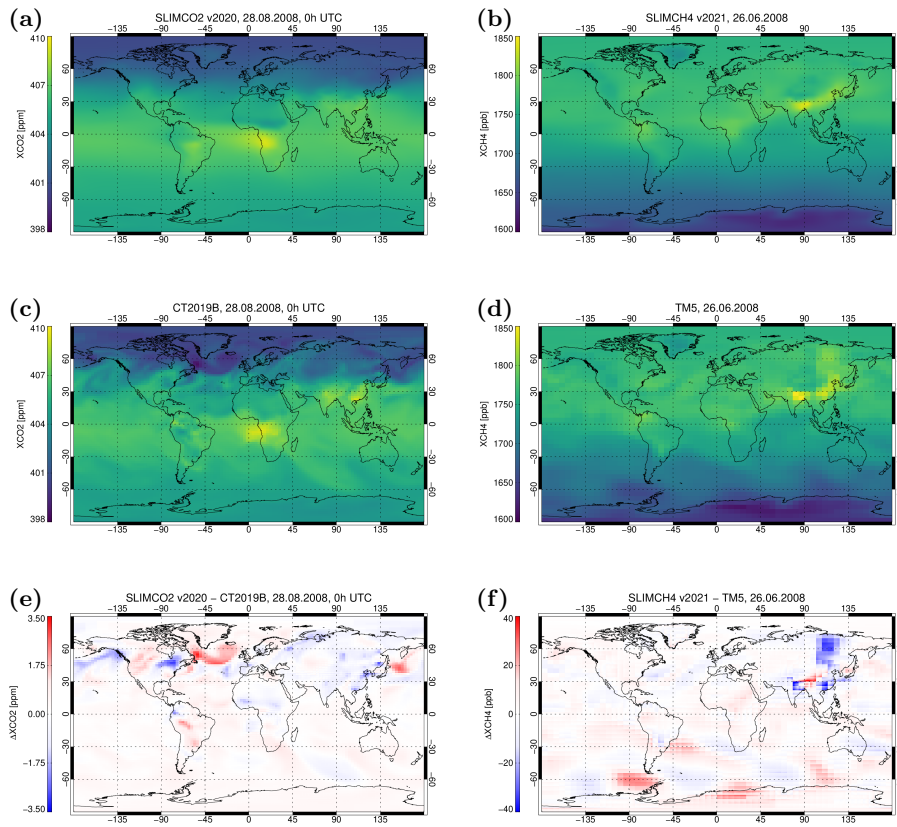
Figure A2. Example Maps of SLIMCO2 (a) and SLIMCH4 (b) data. Panels (c) and (d) show corresponding data from the underlying models (CT2019B, TM5). The differences between the SLIM results and these model data are shown in panels (e) and (f).
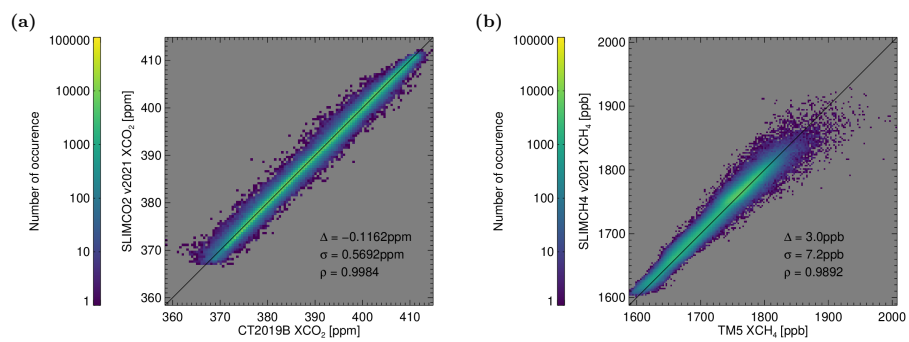
Figure A3. Scatter plot of the data shown in Fig. A2. (a) SLIMCO2 data vs. CT2019B. (b) SLIMCH4 vs. TM5. σ corresponds to the standard deviation of the difference δ corresponds to the average bias, and ρ is the Pearson correlation coefficient.
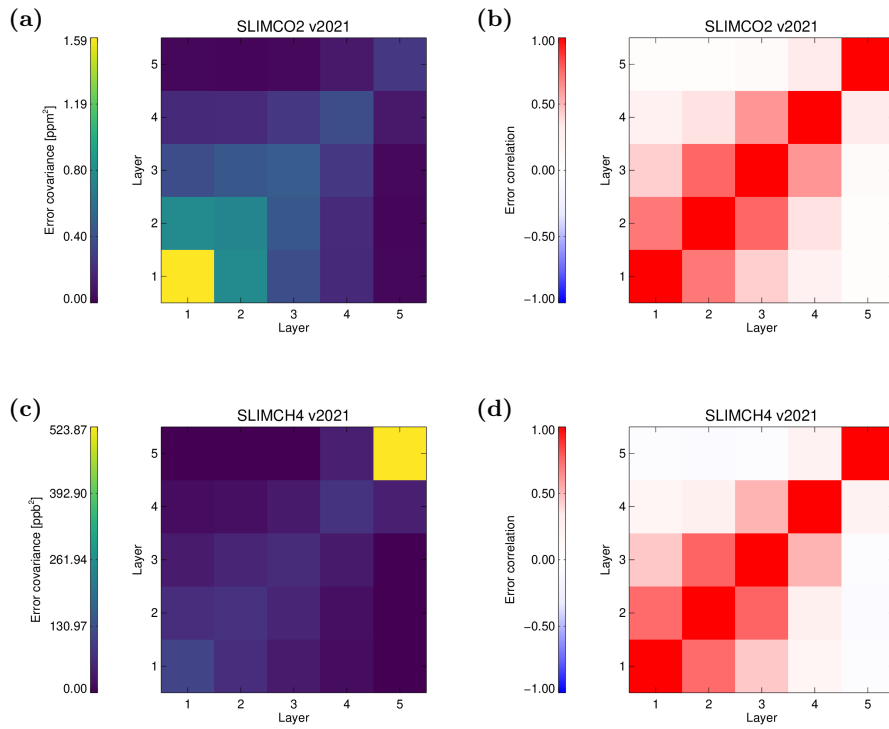
Figure A4. Error covariance matrices for SLIMCO2 (a) and SLIMCH4(c) and corresponding error correlation matrices (b, d).

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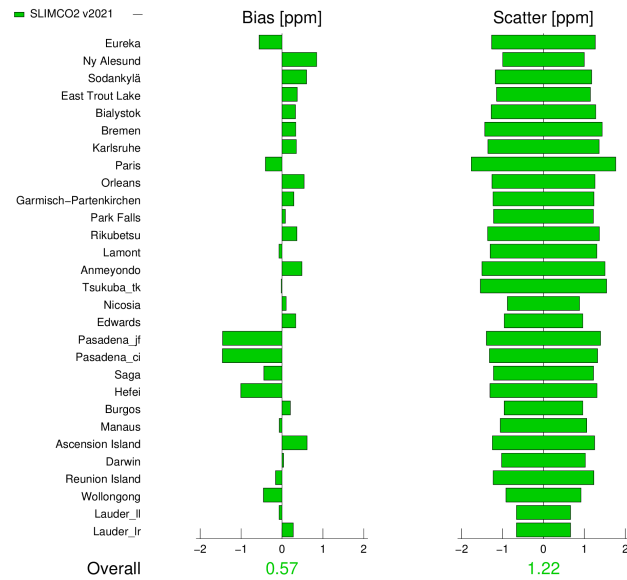
(b)
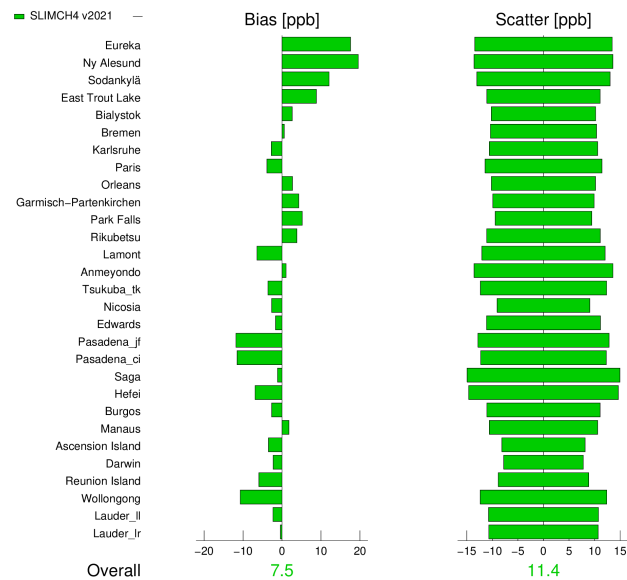
Figure A5. Overview of TCCON validation results for SLIMCO2 (a) and SLIMCH4 (b). The mean station bias has been subtracted to better illustrate the local station differences.

(a)

(b)
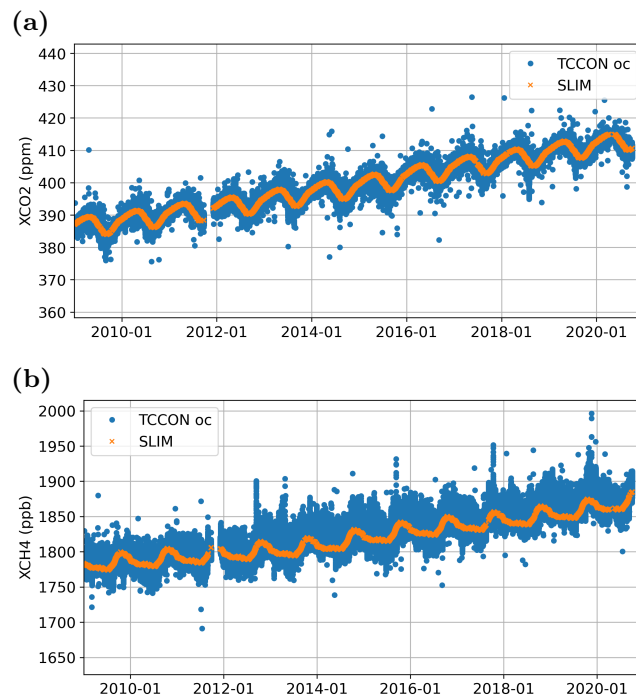
Figure A6. Time series of XCO_2 (a) and XCH_4 (b) from TCCON and SLIM at Lamont (station code oc).
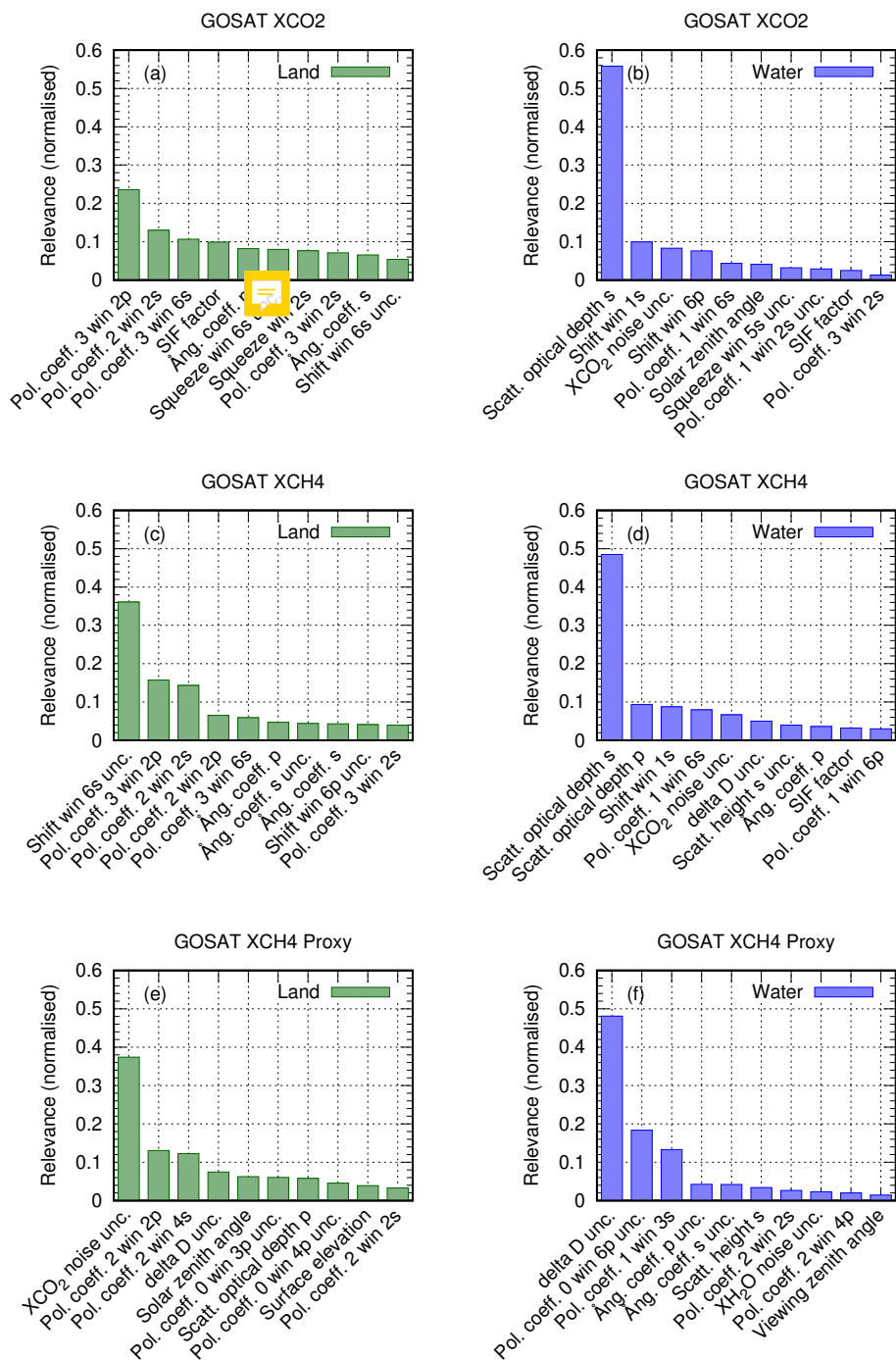
Figure A7. Variables selected for the GOSAT random forest bias correction and their relevance. Top: XCO_2. Middle: XCH_4. Bottom: XCH_4 Proxy. Left/right: For land/water surface.
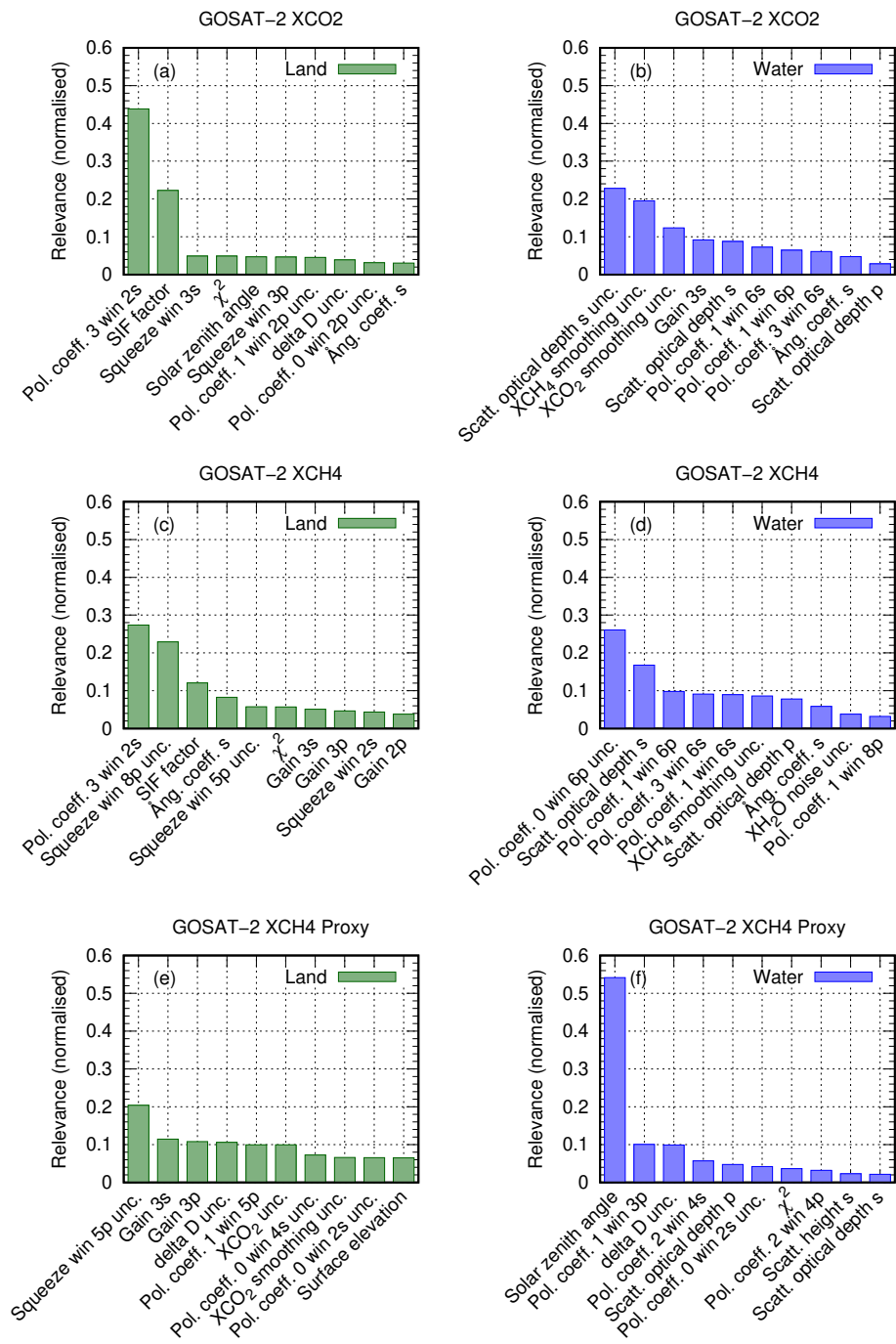
Figure A8. Same as Fig. A7, but for GOSAT-2.

Table A1. XCO$_2$ 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	$1.09\ 10^{-3}$	$5.37\ 10^{-2}$	Scatt. optical depth p	$-7.28\ 10^{-2}$	$3.53\ 10^{-2}$
Scatt. optical depth p	$-5.09\ 10^{-3}$	$2.80\ 10^{-2}$	Scatt. optical depth s	$4.40\ 10^{-3}$	$5.76\ 10^{-2}$
Pol. coeff. 3 win 2s	$-6.98\ 10^{-3}$	$-6.42\ 10^{-5}$	Pol. coeff. 3 win 2s	–	$1.87\ 10^{-3}$
Pol. coeff. 3 win 2p	$-7.32\ 10^{-3}$	$2.91\ 10^{-4}$	XCO$_2$ noise unc. (ppm)	0.58	1.45
Surface roughness (m)	–	54.00	Pol. coeff. 1 win 6p	$2.66\ 10^{-4}$	–
XCH$_4$ noise unc. (ppm)	$3.89\ 10^{-3}$	$6.58\ 10^{-3}$	Pol. coeff. 1 win 5p	$8.01\ 10^{-4}$	–
Scatt. Ångström coeff. p	1.07	–	Pol. coeff. 1 win 5s	$7.67\ 10^{-5}$	–
Spectral squeeze win 3p	$-1.20\ 10^{-3}$	$1.21\ 10^{-3}$	Pol. coeff. 0 win 3s unc.	–	$3.05\ 10^{-4}$
Pol. coeff. 1 win 4s	$-1.46\ 10^{-2}$	$-3.05\ 10^{-3}$	Pol. coeff. 0 win 4p unc.	–	$4.50\ 10^{-4}$
Spectral squeeze win 3s	$-1.21\ 10^{-3}$	$1.24\ 10^{-3}$	δD unc. (per mille)	–	391.41
Pol. coeff. 1 win 6s	$-3.62\ 10^{-3}$	–	Pol. coeff. 0 win 5s unc.	–	$5.72\ 10^{-4}$
Scatt. Ångström coeff. s	$-8.71\ 10^{-2}$	–	χ^2	–	1.02

Table A2. XCH_4 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	$-6.59\,10^{-3}$	$3.45\,10^{-2}$	Scatt. optical depth p	$-7.28\,10^{-2}$	$3.52\,10^{-2}$
Scatt. optical depth p	$2.00\,10^{-3}$	$2.80\,10^{-2}$	Scatt. optical depth s	$4.40\,10^{-3}$	$7.55\,10^{-2}$
Pol. coeff. 3 win 2p	$-7.32\,10^{-3}$	$4.12\,10^{-4}$	Pol. coeff. 3 win 2p	$-8.80\,10^{-3}$	$9.59\,10^{-5}$
Scatt. Ångström coeff. p unc.	0.16	–	Pol. coeff. 1 win 5p	$7.97\,10^{-4}$	–
Surface roughness (m)	–	55.00	Pol. coeff. 1 win 6p	$2.23\,10^{-4}$	$4.51\,10^{-3}$
Pol. coeff. 3 win 2s	$-6.98\,10^{-3}$	$4.90\,10^{-4}$	Pol. coeff. 0 win 2p unc.	–	$5.32\,10^{-4}$
Pol. coeff. 1 win 4p	–	$-4.85\,10^{-3}$	Pol. coeff. 1 win 5s	$4.26\,10^{-5}$	–
Pol. coeff. 1 win 4s	$-1.46\,10^{-2}$	$-4.99\,10^{-3}$	Pol. coeff. 0 win 5p unc.	$5.98\,10^{-5}$	$3.61\,10^{-4}$
Spectral squeeze win 5s unc.	$2.02\,10^{-4}$	$3.99\,10^{-4}$	Pol. coeff. 0 win 3s unc.	–	$2.63\,10^{-4}$
Pol. coeff. 1 win 6s	$-3.79\,10^{-3}$	–	XCO_2 noise unc. (ppm)	0.58	1.47
Scatt. Ångström coeff. s unc.	0.14	1.00	Pol. coeff. 0 win 5s unc.	–	$5.88\,10^{-4}$
Spectral squeeze win 3p	$-1.50\,10^{-3}$	$1.61\,10^{-3}$	Pol. coeff. 1 win 6s	$4.83\,10^{-5}$	$4.53\,10^{-3}$

Table A3. XCH_4 Proxy 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
Pol. coeff. 1 win 4s	–	$-4.11\,10^{-3}$	XCO_2 smoothing unc. (ppm)	–	1.21
XH_2O noise unc. (ppm)	–	20.08	Spectral shift win 3p unc.	–	$1.29\,10^{-3}$
XCH_4 noise unc. (ppm)	–	$1.48\,10^{-2}$	XCO_2 unc. (ppm)	–	5.14
χ^2	–	0.97	XCO_2 noise unc. (ppm)	–	2.40
Spectral squeeze win 5s unc.	–	$5.93\,10^{-4}$	Pol. coeff. 0 win 4p unc.	$7.16\,10^{-5}$	$5.98\,10^{-4}$
Scatt. optical depth p	-0.24	0.13	Pol. coeff. 2 win 4p	–	$1.00\,10^{-4}$
Spectral squeeze win 3p	–	$1.67\,10^{-3}$	Pol. coeff. 0 win 2s	$3.64\,10^{-2}$	–
Pol. coeff. 0 win 6p unc.	–	$1.04\,10^{-3}$	δD unc. (per mille)	–	183.57
Pol. coeff. 1 win 2p	$-7.56\,10^{-3}$	$4.48\,10^{-2}$	Scatt. Ångström coeff. s unc.	$4.11\,10^{-2}$	1.00
Pol. coeff. 1 win 4p	–	$-3.95\,10^{-3}$			

Table A4. XH_2O 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.	$6.25\,10^{-4}$	–	XH_2O noise unc. (ppm)	–	30.47
Pol. coeff. 2 win 6p unc.	$7.21\,10^{-5}$	–	Pol. coeff. 0 win 6p unc.	$1.61\,10^{-4}$	–
Pol. coeff. 0 win 2s unc.	$1.34\,10^{-4}$	–			
Pol. coeff. 0 win 5p unc.	$8.71\,10^{-5}$	–			

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	$1.37\,10^{-2}$	–	Scatt. optical depth s	$1.34\,10^{-2}$	$6.77\,10^{-2}$
δD unc. (per mille)	–	36.02	Scatt. optical depth p	$1.48\,10^{-2}$	$6.18\,10^{-2}$
XH_2O noise unc. (ppm)	7.27	62.48	δD unc. (per mille)	–	38.89
XH_2O unc. (ppm)	8.25	64.63	XH_2O noise unc. (ppm)	9.29	104.62
SIF factor unc.	0.43	–	Pol. coeff. 1 win 1p unc.	$3.22\,10^{-4}$	$1.09\,10^{-3}$
Pol. coeff. 1 win 6p	$-9.43\,10^{-3}$	$1.65\,10^{-2}$	Pol. coeff. 1 win 6s	$-9.81\,10^{-3}$	$3.66\,10^{-3}$
Spectral squeeze win 2s unc.	$3.58\,10^{-4}$	$6.12\,10^{-4}$	Pol. coeff. 1 win 6p	$-3.13\,10^{-3}$	$3.58\,10^{-3}$

Table A6. XCO_2 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. XCH$_4$ 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	$1.91\,10^{-2}$	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. XCH_4 Proxy filter variables and limits for GOSAT-2. "–" means that no limit is applied.

Land Variable	valid range min.	valid range max.	Water Variable	valid range min.	valid range max.
Solar zenith angle (deg)	0.00	75.00	Solar zenith angle (deg)	0.00	75.00
XH_2O 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.	–	$3.35\ 10^{-4}$
XH_2O noise unc. (ppm)	–	16.64	Pol. coeff. 0 win 8p	$3.32\ 10^{-2}$	–
Pol. coeff. 0 win 4p unc.	–	$1.03\ 10^{-3}$	Pol. coeff. 0 win 4s unc.	–	$5.96\ 10^{-4}$
Pol. coeff. 0 win 3s unc.	$5.97\ 10^{-5}$	$3.55\ 10^{-4}$	XH_2O noise unc. (ppm)	–	39.77
Pol. coeff. 0 win 4s unc.	$4.53\ 10^{-5}$	$2.49\ 10^{-4}$	Pol. coeff. 2 win 6s	$-3.26\ 10^{-4}$	$3.78\ 10^{-3}$
Spectral shift win 5s	$-6.64\ 10^{-2}$	–	Scatt. Ångström coeff. s unc.	$3.33\ 10^{-2}$	1.00
Spectral shift win 1p	-0.14	–	Pol. coeff. 1 win 2s	$-9.51\ 10^{-4}$	$3.20\ 10^{-2}$
Pol. coeff. 1 win 2s	$-5.63\ 10^{-3}$	–			
Spectral squeeze win 8p	–	$1.12\ 10^{-3}$			

Table A9. XH_2O 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.	$1.18\,10^{-4}$	–	XH_2O noise unc. (ppm)	–	33.31
χ^2	0.78	–	Pol. coeff. 0 win 3s unc.	$8.84\,10^{-5}$	–
Pol. coeff. 0 win 4s unc.	$6.86\,10^{-5}$	–	Pol. coeff. 2 win 6p unc.	$4.66\,10^{-5}$	–
Surface roughness (m)	–	177.00	XCH_4 smoothing unc. (ppm)	$7.52\,10^{-4}$	$3.70\,10^{-2}$
Pol. coeff. 0 win 2s unc.	$9.89\,10^{-5}$	–	Scatt. Ångström coeff. s	0.71	9.62

Table A10. δD 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	$7.70\,10^{-3}$	–	Scatt. optical depth p	$1.60\,10^{-2}$	$7.64\,10^{-2}$
δD unc. (per mille)	–	30.24	Scatt. optical depth s	$8.81\,10^{-3}$	$5.14\,10^{-2}$
XH_2O noise unc. (ppm)	6.58	52.74	δD unc. (per mille)	–	27.86
XH_2O unc. (ppm)	7.12	53.71	XH_2O noise unc. (ppm)	6.78	125.86
SIF factor unc.	0.34	1.03	Pol. coeff. 3 win 2p	$-6.47\,10^{-3}$	$1.57\,10^{-3}$
Spectral squeeze win 2s unc.	$3.00\,10^{-4}$	$5.42\,10^{-4}$	Pol. coeff. 1 win 2s unc.	$8.97\,10^{-5}$	$3.38\,10^{-4}$
Pol. coeff. 1 win 6s	$-4.01\,10^{-3}$	$3.76\,10^{-3}$			

Table A11. XCO 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. Ångström coeff. s unc.	$5.45\,10^{-2}$	–	XCO unc. (ppm)	–	$8.60\,10^{-3}$
Pol. coeff. 1 win 5s	$-1.27\,10^{-2}$	$2.19\,10^{-3}$	Pol. coeff. 1 win 2s	$7.57\,10^{-4}$	$3.50\,10^{-2}$
Pol. coeff. 2 win 5s	$-1.06\,10^{-3}$	–	XH_2O noise unc. (ppm)	–	22.72
Scatt. Ångström coeff. p unc.	$6.13\,10^{-2}$	–	Pol. coeff. 0 win 7s unc.	$5.40\,10^{-5}$	–
Pol. coeff. 1 win 2s	$-5.80\,10^{-3}$	–	Scatt. height s unc.	$4.99\,10^{-3}$	–
XCH_4 smoothing unc. (ppm)	$7.99\,10^{-4}$	–	Pol. coeff. 2 win 7s unc.	$1.41\,10^{-4}$	–
XCO unc. (ppm)	–	$9.62\,10^{-3}$	Scatt. Ångström coeff. s unc.	$3.76\,10^{-2}$	–

Table A12. XN_2O 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_2O 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_2O 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	$2.15\,10^{-3}$	–