XCO$_2$ retrieval for GOSAT and GOSAT-2 based on the FOCAL algorithm

by S. Noël et al.

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Authors' Response

Reply to referee 1

We thank the referee for the review and the constructive 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 and the proposed updated text for the revised version of the manuscript in **bold** font.

Answers to General comments:

1. *Overall, I found this paper useful and interesting, and will serve as an important reference. The subject matter is important, the layout of the paper is logical, the reasoning sound, and the results are generally laid out well. However, there are a number of problems that need to be addressed. While details of the retrieval, filtering, and bias correction were presented in a straightforward way, it was quite dry with little learned. Especially in the part about the random forest filter, which was used for both filtering and bias correction, but with little attempt on the part of the authors to explain the relevance of the features identified. The same goes for the prefilters, where it appeared that thresholds were drawn somewhat out of thin air for some of the parameters. It would have been useful if the authors had shown even a couple example plots of some of the prefilters and how thresholds were determined.*

   Regarding random forest filtering, the relevance of the different features is determined by the random forest method and shown in Figs. 7 and 8. A physical explanation of these relevances is not possible – this is a general problem of this method. Therefore we think that plotting individual maps of parameters is not helpful here.

   There is indeed no well defined procedure to define the prefilters, this is essentially based on "scientific knowledge", e.g. trying to set (in a physical sense) reasonable limits for some parameters. Therefore – as written in the paper – the choice of the XCO2 error limit or the maximum optical depths of the scattering layer is somewhat arbitrary and essentially based on trying out different values and looking at the resulting scatter of the data after filtering. It is therefore not possible to show e.g. a single example map of one of these parameters from which the limits can be derived. or justified.

   We are aware of this problem, and for future product versions we will try to improve the filtering method.

2. *There were 25 figures in this paper, and in my opinion, many more than are useful, especially some of the earlier plots. I suggest the authors try to remove some panels in some plots, or some plots altogether, to show representative plots. For instance, all the noise model coefficients are given in Tables 6 & 7. Therefore, the authors can reduce Figs 3-6 to probably a single 2 or 4 panel plot (e.g., Fit Windows 2 & 3 for both GOSAT and GOSAT-2, P-polarization only). The same goes for Figs 9-12 (a single one would do) and Figs 13-16 (again, a single one would do, and not all bands are necessary). Plots are in the paper to explain findings, not to exhaustively present ever detail of the study, especially if some plots or features of plots are never discussed in the main body of the paper.*

We agree and will combine / remove plots to reduce the number of plots accordingly. For the noise model we will show windows 2P (O2 band) and 6P (strong CO2 band) for both GOSAT and GOSAT-2 in one figure. Spectra and residuals will be combined into one plot, and we will only show P polarisation, so there will be one plot for GOSAT and one for GOSAT-2.

3. *Finally, it appeared that many important previous works by other authors are never referenced, or included in the reference section but never cited in the main body. In general, referencing needs to be much improved in this work.*

   We will include additional references as suggested by the referee and also check existing references.

4. *Therefore, I recommend publication of this manuscript after a major revision to fix the issues with the burdensome # of plots and problems with referencing, as well as addressing all the specific concerns raised below.*

   See below for our answers to the specific comments.

Answers to Specific comments:

1. *Section 2.3: This is a unique approach to a truth database to my knowledge – it needs more information (plots, etc) on how big this contiguous regions are / how much the TCCON data are expanded through this approach. A map of a month or a season of data density would fulfill this, and I think be very interesting for readers. Otherwise, it's not clear how much this really expands over just using TCCON directly.*

   We will add an example map of the true database.

2. *Section 2.3: Secondly, you say the requirement for contiguous regions, but you never say how close the ak-corrected CT value at the TCCON location & time has to agree with TCCON itself. Is that also 0.75 ppm? You imply this but never say – please correct this.*

   The contents of the "true" database is not selected based on a 0.75 ppm maximum difference to TCCON data but to a subset of CT data at TCCON locations. This subset has been selected as having a maximum difference of 0.75 ppm between the ak-corrected CT value at the location of the station and the TCCON value.

   The "true" database therefore contains only CarbonTracker data, which are confirmed by TCCON measurements but may differ by up to 1.5 ppm from the TCCON value. This is explicitly stated in the manuscript at the end of this section:

   "Please note that the "true" database does not contain any TCCON data - it only contains CT data which were confirmed by TCCON, but individual values may differ by up to 1.5 ppm."

   We will clarify this in the text.

   We also decided to rename the "true database" to "reference database" to indicate that the content is not necessarily the (essentially unknown) "true" XCO2 at a certain time and place but only an estimate which should on average reproduce large scale features correctly.

3. *Section 3.1: Your terms "cloud albedo" and "water vapor path" are neither. These terms already have definitions in use by the community, and they are not how you define them. I suggest you rename "cloud albedo" to "effective albedo" or "effective scene albedo". Note you will screen out some bright desert scenes with your albedo filter, though probably not many. It looks like your 1.98 μm filter is doing most of the work. Regarding "water vapour path", it's nothing of the sort. It's more like an SNRwv(wv="water vapour"), or SNR 1.93 (since this band is roughly at 1.93 μm). Low SNRwv= clear, high SNRwv= cirrus present. So please rename it to something else.*

   We agree that the nomenclature we used here is misleading. We will therefore replace "cloud albedo" by "effective albedo" and will rename "water vapour path" to "water vapour filter" to clarify this. The albedo filter may indeed remove scenes with very high surface albedo, but this seems to be uncritical in our case as we still have data over deserts after cloud filtering.

4. *Section 3.2 – Please MOTIVATE why you use both polarisations separately. Do you believe you obtain more information than if you averaged them together, or do you believe you cannot accurately average because certain instrument properties (such as ILS) are different for the two polarisations, and they themselves cannot be averaged together?*

   We use both polarisation corrections mainly for the following reasons:

   - In principle, information is lost when averaging S and P spectra.
   - In general, the sensitivity of the instruments and therefore the calibration of the measured spectra is different for S and P. For example, as mentioned by the referee, the measured ILS is given independently for S and P.
   - S and P include different information on scattering, which can also be used for filtering and/or bias correction.

   We will mention this in the paper.

5. *Section 3.2.1 Near line 263, you talk about the "NIR", but early in the paper you refer to ALL the bands you use as "SWIR". I realize most scientists label the O2A band as NIR and everything past 1 micron as SWIR. Can you please go through the paper and ensure consistency between NIR and SWIR labels throughout?*

   We will harmonise the use of "NIR" and "SWIR" in the revised version of the paper.

6. *Section 3.2.1 – Way too many plots, as I said in the general comments. As a rule of thumb, try not to overwhelm readers with a bunch of plots that all look essentially the same. Each panel of each plot should contribute to the story you are telling.*

   We agree and will remove / combine figures as suggested.

7. *Section 3.3.1 – In general, your "basic filter" through the RSR filters (I'm looking at your figures 1-2 for this information) really does seem basic for GOSAT, as it filters out only 8 percent of the data (35.0%–>27.2%), and most of that comes from convergence. However, for GOSAT-2 not only do twice as many soundings fail to converge as for GOSAT, but the window 5 RSR also accounts for many failed soundings (5% for GOSAT-2, versus 0.3% for GOSAT, if I am counting right). Can you please comment on why this may be happening for GOSAT-2? Window 5 is the methane band I think. You may wish to split things out separately as land versus ocean – you may find very different behaviors for the two categories. In any event, please devote a few words in this section as to why this is happening. And please do say how differently the filters act on land vs. ocean. Actually, looking at this further, I think it is the "broadband oscillation" in the fit residuals you mention for GOSAT-2 that may be causing the problem. Are those oscillations really correlated with retrieved XCO2 quality? If not, you may wish to loosen that constraint for GOSAT-2, to save more soundings.*

   We use the term "basic filter" for all post-processing filters applied before the random forest filter. Indeed, the number of data removed by the RSR filter is much larger for GOSAT-2 than for GOSAT. We assume that this is mainly related to the GOSAT-2 calibration which e.g. currently does not consider remaining polarisation sensitivities to the U (45°) component of incoming light, which especially affects band 2 and may be the reasons for the broadband features in window 5.

   Furthermore, as explained in the paper, there seem to be some problems with the noise of GOSAT-2 data over water, which is why we base our GOSAT-2 noise model on land data only. This is also why we cannot provide separate RSR filters for land and ocean for GOSAT-2. For GOSAT different RSR filters are not necessary as there is no discrepancy in the land/ocean noise data. This is why we apply the same convergence / RSR filters for land and water (but later split the filtering and bias correction).

   We rely on the calibrated spectra given in the data product and thus cannot quantify the real impact of the deficiencies in the calibration on the retrieval results. We therefore prefer not to add speculations about possible reasons to the paper.

However, the different performance of the filters indicates that the filtering for GOSAT-2 needs some further optimisation, which is planned for the next version of the products.

We will mention the latter in the paper.

8. *Secton 3.3.2 Near line 295, please also reference Mandrake et al (2013, AMT, "Semi-autonomous sounding selection for OCO-2"), who did something similar for OCO-2.*

   We will add this reference.

9. *Section 3.3.2, near line 310. I'm nearly certain that for water, SAA, VAA, SZA, VZA will be correlated with latitude. Because the orbit is sun-synchronous and you're looking to the glint spot over water, I'm willing to bet that any machine learning algorithm or even a simple correlation analysis can probably figure out where you are based on those quantities (or even only one or two of them). I suggest you be exceedingly careful in including those quantities. Please include a comment to this affect in the paper.*

   We agree that for water / glint there are specific relations between viewing geometry and geolocation and will mention this in the paper.

10. *Section 3.3.2 – can you state how many training soundings total there were for GOSAT and GOSAT-2, for each of land and water? I wonder if your training set is general enough to avoid over-fitting. Also, please define "Relevance" as you use it in Figure 7 & 8.*

    The number of soundings used for the random forest filter are:

    - GOSAT land: 54317
    - GOSAT water: 109414
    - GOSAT-2 land: 10625
    - GOSAT-2 water: 40459

    From these, we use 90% for training and 10% for testing, so this should be sufficient for 10 parameters. We think that over-fitting is not a problem here, because as mentioned in the paper we only get accurate filter results in two thirds of the cases (for both training and test data sets). This would not be the case for over-fitting where the training set would have a much better performance than the test data set.

    "Relevance" is a quantity coming out of the random forest method which describes the relative importance of each feature for the filtering. Relevances are normalised such that the sum of all relevances is 1.

    We will include this information in the paper.

11. *Section 3.3.3 – This community did XCO2 bias correction long before OCO-2. Can you please reference earlier works on the subject? (The earliest I know of is Wunch et al., 2011, ACP "A method for evaluating bias..."; I believe there are similar references for GOSAT for the UoL retrieval, the NIES retrieval, and the RemoTeC retrieval). Are you really using 10 parameters in your bias correction? This is way more than most groups usually use (which is typically 1-4; as I remember, Reuter et al.(2017) didn't use any in their OCO-2/FOCAL paper). Be careful – there could almost certainly be overfitting here. So my comment is 10 parameters simply doesn't seem to be justified based on past experience and the published methods of nearly all other retrievals for the last 10 years. Therefore, your using 10 parameters requires more justification than simply "this is what came out of the random forest algorithm".*

    We will add additional references to other bias correction methods.

    The choice of filter parameters is mainly based on the output of the random forest method, which associates to all possible parameters a relevance value (shown e.g. in the top of Fig. 7 for GOSAT). As explained above, this relevance value describes the relative importance of a suggested feature for the filtering or regression. As can be seen from this figure, the relevance drops off quite rapidly

after a few variables. The number of variables to be used is then a trade-off between many variables (explaining all relations with a risk for over-fitting and high computational effort) and few variables (no over-fitting, but maybe missing some relations). We decided to use 10 variables as a good compromise, and since we do not seem to have problems with over-fitting (see answer to previous comment) this seems justified. Note that even if we would include too many non-relevant parameters, this would be no major problem as most filtering is done by the relevant parameters.

We will include this explanation in the paper.

12. *Section 4, nearly line 378. Just a comment. The higher XCO2 variability over land has long been seen. I highly doubt this is due solely to surface variability. I think it is also caused by different scattering pathways that are not present over water. In particular, photons scattered downward by the atmosphere can be reflected off the surface back into the beam accepted by the sensor; this mechanism doesn't happen over water, so there are more ways for atmospheric scattering to degrade a retrieval. But that's mainly just a hypothesis.*

Thank you for the information. We agree that surface variability may not be the only reason for the higher XCO2 variability over land. We will adapt the text accordingly and take your comment into account.

13. *Section 5 – page 13. Please include appropriate references for each of these algorithms here. Also you say for the validation of the GOSAT and GOSAT-2 FOCAL products, but really these comparisons to the other products are just for GOSAT only. You may wish to state upfront here that the vast majority of the presented validation is only for GOSAT. Only subsection 5.3 mentions GOSAT-2, and it only appears in a single validation figure (25). In fact, this paper is really begging for some basic comparison plots of GOSAT and GOSAT-2 to TCCON, to see how well your algorithm works on GOSAT-2 as compared to GOSAT. Can you please add something to that effect?*

Detailed references for all products are already given in Section 2.4. Indeed, most comparisons are done for GOSAT, except for the time series (section 5.3).

We did not include a comparison of GOSAT-2 with TCCON because of the limited amount of the GOSAT-2 data. We will add this in the revised version but note also that the results are probably not representative.

14. *Line 438 – I do not understand this statement about a "bias anomaly". Please be more clear about what you did here. Did you subtract some kind of mean bias with respect to TCCON from each algorithm? Please don't! Or if you did, you have to state somewhere what number you subtracted off each algorithm. If ACOS is high by 1 ppm relative to TCCON and you simply subtracted that off before making plots, it's critical to state that somewhere. It would be much better simply to NOT subtract off that bias, unless you can throughly justify why you did.*

We subtracted for each algorithm the mean of the bias for all stations. This is because for most applications this mean bias is not relevant since most information is contained in gradients. Subtracting a mean bias also facilitates a comparison of different bias patterns between the algorithms.

The subtracted mean station bias is actually small (0.17 – 0.64 ppm). We will mention this in the paper.

15. *Section 5.2 end, L445 – Even if you don't have "sufficient data" for full seasonal cycle fits for all GOSAT-2 data vs. TCCON, you've got enough to make some basic plots. Please do so – the community is really interested in them. If not, there isn't a lot of point in including GOSAT-2 in this paper at all.*

As mentioned above, we will include some plots for GOSAT-2 vs. TCCON.

16. *References: It looks like you have way more references in the Reference section of the paper, than you actually reference in the main body of the paper. A rule of papers: you MUST cite each reference in your references section somewhere in the main body of the paper. Please make sure this is the case.*

We will check the references, but actually all entries in the References section are cited in the paper. However, the references for the used TCCON data are only listed in Table 1, maybe this is why the referee misses them in the main text.

Answers to Technical/Grammatical comments:

1. *47: Tansat, GOSAT, and OCO-2/3 instruments The Tansat, GOSAT, and OCO-2/3 instruments*

   Will be corrected.

2. *L280: XCO2 error is ambiguous. Suggest you change this to "XCO2 posterior uncertainty" or something more clear that it is the posterior error estimate from the OE itself, and not some error as compared to TCCON or something.*

   Agreed, will be changed.

3. *L292: Remove the word "exemplary". This isn't really an example, I assume this is a full indication of what is happening.*

   Indeed, "exemplary" may not be the correct term here. However, the figures only show an example for one month of data (as written in the caption). We will rephrase this sentence:

   Figs. 1 and 2 show how many data points are typically filtered out in this step.

   Note: The numbering of figures above refers to the current paper, it will change in the revised version.

Reply to referee 2

We thank the referee for the detailed review. The comments 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 and the proposed updated text for the revised version of the manuscript in **bold** font.

Answers to major comments:

1. *Section 2.3 "True database"*

   (a) *It remains unclear whether the actual TCCON measurements are used or not in the procedure. My current understanding is that the "valid" simulations are those where the total column, computed with an homogeneous weighting and the same with the TCCON averaging kernel, differ by less than 0.75 ppm. If my understanding is correct, then (i) I do not understand why this is a valid criterium to select the most accurate simulation data and (ii) there is no need to compute the "daily mean" TCCON. If my understanding is incorrect, the description needs some re-writing.*

   For the "true" database we first determine a set of daily TCCON data for each station. These TCCON data are an average over all measurements within $13\,\text{h} \pm 2\,\text{h}$ local time of one day at one station. This is no daily mean as it is only a 4 h average (we'll clarify this in the paper). From this, we get one value per day and station. We then select collocated CarbonTracker (CT) data for each day and station, apply the TCCON averaging kernels to them and compute XCO2. This ak-corrected CT XCO2 is then compared with the corresponding TCCON XCO2. For all days where both values agree within $\pm\,0.75$ ppm, we define contiguous regions around each station where the CT XCO2 data deviate less than 0.75 ppm from the CT value at the station. The CT data inside these regions are then inserted into the database.

   The "true" database therefore contains only CT data, which are confirmed by TCCON measurements but may differ by up to 1.5 ppm from the TCCON value. This is explicitly stated in the manuscript at the end of this section:

   "Please note that the "true" database does not contain any TCCON data - it only contains CT data which were confirmed by TCCON, but individual values may differ by up to 1.5 ppm."

   The choice of the 0.75 ppm ranges is based on a trade-off between accuracy (agreement with TCCON) and spatial coverage of the database.

   We will update the section about the "true" database for clarification.

   (b) *Line 138-139 "which were confirmed by TCCON" is really unclear, especially since it is said above that there is "more data in the Southern hemisphere" that is notably poor in TCCON coverage. How can such data be confirmed by TCCON.*

   As explained above, "confirmed by TCCON" means that all CarbonTracker data used in the "true" reference database agree within 1.5 ppm with TCCON. This essentially defines an area around each used TCCON station where CarbonTracker data are compliant with this criterion. The spatial coverage of the "true" database varies from day to day depending on how many data agree with TCCON. This of course also limits the spatial coverage of the "true" database (e.g. there are less data in the southern hemisphere), but nevertheless all data in the "true" database fulfil the criterion and are therefore confirmed by TCCON.

   The sentence "There are typically more data in the southern hemisphere during the second half of the year" just means that there are more data during the second half of the year compared to the first half of the year, not more data in the south than in the north. We will clarify this in the text and also show example maps from the "true" data base to illustrate this.

   (c) *As a consequence, it is really unclear why the database build as described, can be considered as a truth.*

For the XCO2 bias correction we have to assume some kind of "truth", and we think our choice to use a subset of CarbonTracker data which is confirmed by measurements is a valid one. We hope that with the explanations given above this is now clearer.

We also decided to rename the "true database" to "reference database" to indicate that the content is not necessarily the (essentially unknown) "true" XCO2 at a certain time and place but only an estimate which should on average reproduce large scale features correctly.

2. *Section 3.1.2 Cloud Filter*

   *It is said that the Cloud Filter is based on the fact that clouds are bright (OK) and higher in the atmosphere so that there is little water vapour above them. Then, one my expect that, when the water vapor estimate is low, a cloud presence is suspected. Yet the description of the test indicates that a cloud is detected when the water vapor estimates is **larger** than a threshold. This is inconsistent.*

   The referee is completely right. The term "water vapour path" which we use to name one of the filter criteria for cloudiness is misleading. As written in the manuscript, this filter is defined as the ratio between the median radiance and the median of the estimated noise, i.e. it is indeed high in case of low water vapour content and vice versa.

   We will rename "water vapour path" to "water vapour filter" to clarify this.

3. *Section 3.3.2 Random Forest Filter*

   (a) *The difference between the estimate and the "true" reference database is used. It is said that the difference is subtracted by the global monthly mean bias. This assumes that the global mean bias of the reference is zero which is a strong assumption.*

   As written in the manuscript, for the filtering we are not interested in a potential global bias of the data. The main purpose of the random forest filter is to reduce the scatter in the XCO2 data. This is why we subtract the global median of the bias before filtering. It is indeed the global median for land and water, not the monthly global median, which is subtracted – this will be corrected in the paper. This essentially makes the filtering independent from a global bias.

   For the bias correction, however, we assume that our reference (the "true" database) is on average the "truth", i.e. large scale features are well reproduced. This is indeed a strong assumption, but this is how a bias correction works, and we think we made a reasonable choice for the reference.

   (b) *This section lacks a quantitative discussion: What are the mean values of the differences to the "true" reference dataset. What is the order of magnitude of the bias correction? Does it has some spatial patterns. In the case of ACOS, the bias correction is similar to the signal which is an important information. Is it the same here?*

   Note that this section is not about the bias correction, it is about filtering of data. The bias correction is addressed in the following section, which also gives some quantitative information. Finally, we only use data where the estimated bias is within $\pm$ 2 ppm around the global mean bias, which is different for land and water (see Table 9). The scatter (global standard deviation) of the estimated bias is below 1 ppm.

   We will add this information in the paper and also maps of the bias correction for GOSAT and GOSAT-2 such that spatial patterns can be identified.

   (c) *It is then said (line 321) that the random forest classification is accurate in about two thirds of the cases. How is this evaluated? How can one decide whether it is accurate or not?*

   The accuracy is estimated from the performance of the filter for the training and the test data sets (for which we know the truth). It is defined as the fraction of correctly classified samples.

   We will explain this in the updated paper.

4. *Figures*

8

(a) *There is certainly no need for Figure 3 to 6. A couple of examples would be sufficient rather than the 28 pannels that indicate similar behaviors (and differences that are not commented).*

We agree and will replace Figs. 3 to 6 by a single one showing only an example of the noise plots for GOSAT and GOSAT-2 (two fit windows each).

(b) *Figure 9 to 12 provide no usefull information. Figure 13 to 16 could be limited to a few examples rather than the 30 pannels. I strongly recomment to combine figure 9 and 13 so that one can identify whether the fine scale structures of the residuals correspond to absorption lines*

We agree and will replace these figures by two figures (one for GOSAT and one for GOSAT-2) which will show both spectra and residuals in one plot for only one polarisation direction as indeed results for S and P are very similar.

5. *Section 4; Results*

This section contains several hypothetical statements "likely", "most likely", "which may explain"... that deserve investigations

We agree that some of our formulations are too cautious. We will check the text and update it accordingly.

Answers to other comments:

1. *Abstract : Line 21 "regional bias".*

There is no demonstration that TCCON is representative of a region, neither that the bias at the TCCON location is the same over a region.

With "regional bias" we refer to the "station-to-station bias" which is a measure for the variability of the bias between different stations and thus regions. For clarification, we will use the term "station-to-station bias" in the abstract.

2. *Section 2.2; line 111-112*

Why a factor of 5 for H2O "to reduce dependencies on the a-priori" but not the same factor for the CO2

The natural variability of H2O is much higher than for CO2, therefore we use a stronger a-priori constraint for CO2 than for H2O.

3. *Line 117 "very accurate". Please quantify.*

The estimated accuracy of TCCON XCO2 measurements is 0.4 ppm (1 sigma). We will specify this in the text and add a reference.

4. *Line 124 : "daily mean".*

I understand the mean is over 4 hours. How can this be considered a daily men ?

Yes, the mean is indeed over 4 hours (13±2 h LT), we will correct this:

Then we determine from the TCCON data for each day mean values (XCO_2^{TCCON}) for 13 h ± 2 h local time.

5. *Line 188 : "It is given by the ratio between the median radiance and the median of the estimated noise in this spectral range". Unclear.*

This is the definition of the "water vapour path" filter, see also above. We will reformulate this:

This filter is defined as the ratio between the median radiance and the median of the estimated noise in this spectral range.

6. *Line 278 : The case is rejected when the Angstrom coefficient is outside of the range [1 − 5]. This is strange. Clouds and aerosols can have Anstrom coefficients that are close to zero. Conversely, values larger than 2 have never been reported to my knowledge.*

The FOCAL forward model considers only a single Lambertian scattering layer to describe all scattering effects. All retrieved scattering parameters such as Ångström exponent can be considered "effective" parameters as they have to account for not only cloud/aerosol scattering but also Rayleigh scattering (which has an Ångström coefficient of 4). Because Rayleigh scattering is always present and we filter out cloudy scenes, we usually get higher effective Ångström coefficients than those expected from clouds or aerosols only. We will clarify this in the text.

7. *Line 335: "But with this filter applied". Which filter ?*

   The random forest filter, will be clarified:

   For the bias correction we use as input the same data set as for the random forest filter, but with this random forest filter applied.

8. *Line 343 : What is the order of magnitude of the bias correction?*

   This is explained in the following text; values are given in Table 9. We will also add maps of the bias correction, see our answer to the major comments.

9. *Line 349: "On the derived XCO2 bias".*

   What bias is that? Is it before or after the correction? The paragraph indicates it is after correction, but then how can it be evaluated?

   This is the bias estimated via the random forest classifier. We will clarify this:

   These are filtered out by an additional filter on the XCO2 bias derived via the random forest classifier.

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 the attached version of the revised manuscript.

XCO$_2$ retrieval for GOSAT and GOSAT-2 based on the FOCAL algorithm

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Abstract.

Since 2009, the Greenhouse gases Observing SATellite (GOSAT) performs radiance measurements in the near-infrared (NIR) and shortwave-infrared (SWIR) spectral region. From February 2019 onward, data from GOSAT-2 are also available.

We present first results from the application of the Fast atmOspheric traCe gAs retrieval (FOCAL) algorithm to derive
5   column-averaged dry-air mole fractions of carbon dioxide (XCO$_2$) from GOSAT and GOSAT-2 radiances and their validation. FOCAL has initially been developed for OCO-2 XCO$_2$ retrievals and allows simultaneous retrievals of several gases over both land and ocean. Because FOCAL is accurate and numerically very fast it is currently considered as a candidate algorithm for the forthcoming European anthropogenic CO$_2$ Monitoring (CO2M) mission, to be launched in 2025.

We present the adaptation of FOCAL to GOSAT and discuss the changes made and GOSAT specific additions. This includes
10   particularly modifications in pre-processing (e.g. cloud detection) and post-processing (bias correction and filtering).

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A feature of the new application of FOCAL to GOSAT/GOSAT-2 is the independent use of both S and P polarisation spectra in the retrieval. This is not possible for OCO-2, which measures only one polarisation direction. Additionally, we make use of GOSAT's wider spectral coverage compared to OCO-2 and derive not only XCO_2, water vapour (H_2O) and solar induced fluorescence (SIF) but also methane (XCH_4), with the potential for further atmospheric constituents and parameters like semiheavy water vapour (HDO) and (in the case of GOSAT-2) also carbon monoxide (CO) total columns and possibly nitrous oxide (XN_2O).

Here, we concentrate on the new FOCAL XCO_2 data products. We describe the generation of the products as well as applied filtering and bias correction procedures. GOSAT-FOCAL XCO_2 data have been produced for the time interval 2009 to 2019. Comparisons with other independent GOSAT data sets reveal an agreement of long-term temporal variations within about 1 ppm over one decade; differences in seasonal variations of about 0.5 ppm are observed. Furthermore, we obtain a ~~mean regional~~ station-to-station bias of the new GOSAT-FOCAL product to the ground based Total Carbon Column Observing Network (TCCON) of 0.56 ppm with a mean scatter of 1.89 ppm.

The GOSAT-2-FOCAL XCO_2 product is generated in a similar way as the GOSAT-FOCAL product, but with adapted settings. All GOSAT-2 data until end of 2019 have been processed. Because of this limited time interval, the GOSAT-2 results are considered to be preliminary only, but first comparisons show that these data compare well with the GOSAT-FOCAL results and also TCCON.

1 Introduction

Carbon dioxide (CO_2) is the most important greenhouse gas in the context of global warming (e.g. IPCC, 2013). The amount of CO_2 in the atmosphere is primarily determined by natural and anthropogenic sources and sinks but our current understanding of these sources and sinks has significant gaps (e.g., Ciais et al., 2014; Reuter et al., 2017a; Friedlingstein et al., 2019; Janssens-Maenhout et al., 2020). Retrievals of column averaged carbon dioxide (XCO_2) from the satellite sensors SCIA-MACHY/ENVISAT (Burrows et al., 1995; Bovensmann et al., 1999; Reuter et al., 2010, 2011), TANSO-FTS/GOSAT (Kuze et al., 2016) and from the Orbiting Carbon Observatory-2 (OCO-2) satellite (Crisp et al., 2004; Eldering et al., 2017; O'Dell et al., 2012, 2018) have been used in over a decade to obtain information on natural CO_2 sources and sinks (e.g., Chevallier et al., 2014; Chevallier, 2015; Reuter et al., 2014b, 2017a; Schneising et al., 2014; Basu et al., 2013; Houweling et al., 2015; Kaminski et al., 2017; Liu et al., 2017; Eldering et al., 2017; Yin et al., 2018; Palmer et al., 2019) and on anthropogenic CO_2 emissions (e.g., Schneising et al., 2008, 2013; Reuter et al., 2014a, 2019a; Nassar et al., 2017; Schwandner et al., 2017; Miller et al., 2019; Labzovskii et al., 2019; Wu et al., 2020; Zheng et al., 2020)

First satellite measurements of XCO_2 were performed by the Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (SCIAMACHY) instrument (Bovensmann et al., 1999; Gottwald and Bovensmann, 2011; Reuter et al., 2010, 2011) on the European environmental satellite ENVISAT launched in 2002 and operating until April 2012.

Whereas greenhouse gases were only one field of application among others of SCIAMACHY, later satellite missions focused explicitly on these. In 2009, the Greenhouse gases Observing SATellite (GOSAT; Kuze et al., 2009, 2016) was launched,

followed by the Orbiting Carbon Observatory-2 (OCO-2; Crisp et al., 2017; Eldering et al., 2017; O'Dell et al., 2012, 2018) in 2014. Furthermore, in 2016 the Chinese TanSat mission was launched; first results have been presented by Yang et al. (2018). Follow-on instruments to GOSAT and OCO-2 (GOSAT-2; Suto et al., 2020) and (OCO-3; Eldering et al., 2019) are in orbit since 2018 and 2019, respectively. The TanSat, GOSAT and OCO-2/3 instruments are still operating, and several different retrieval algorithms have been developed to derive XCO_2 from their near-infrared (NIR) and short-wave infrared (SWIR) spectra.

The main challenge for space-borne XCO_2 measurements is the required accuracy of the resulting data products as the atmospheric background of XCO_2 is high compared to the variability, which is typically less than a few percent (about 2% seasonal cycle variations in the northern hemisphere in addition to an annual increase of about 0.5% per year, see e.g. Schneising et al., 2014; Buchwitz et al., 2018). Depending on the application, even higher accuracies are needed. An accurate XCO_2 retrieval usually requires a complex retrieval method and large computational effort. This is no major problem for the number of measurements provided by the GOSAT instruments, but even current OCO-2 retrievals require significantly larger computational effort. However, new missions with much higher spatial resolution and coverage are currently in preparation to answer the challenging questions on CO_2 local and global sources and sinks in a changing climate, one amongst them is the forthcoming European anthropogenic CO_2 Monitoring (CO2M) mission (Kuhlmann et al., 2019; Janssens-Maenhout et al., 2020), dramatically increasing the computational power needed for retrievals.

Three years ago, Reuter et al. (2017b, c) developed the Fast atmOspheric traCe gAs retrieval (FOCAL) and applied it to OCO-2 data. To show the applicability of the FOCAL method not only to OCO-2 but also to other satellite sensors, we present in this study a new application of FOCAL to GOSAT and also some first results from an application to GOSAT-2. GOSAT-FOCAL has several advantages over GOSAT-BESD (Heymann et al., 2015), the currently used IUP GOSAT ~~XCO2~~ XCO_2 retrieval, product (Heymann et al., 2015), which provides only XCO_2 data over land. However, FOCAL is able to retrieve not only XCO_2 but – depending on the used spectral ranges – also other atmospheric parameters like XCH_4, H_2O, HDO, CO and N_2O. In the present study we concentrate on XCO_2, as this is the most important (and because of its high requirements on accuracy possibly most challenging) anthropogenic greenhouse gas.

The manuscript is organised as follows: In Section 2 we list all data sets used in this study. The retrieval algorithm is described in section 3. Sections 4 and 5 then show the results of the retrieval and the validation. Finally, the conclusions are given in section 6.

2 Data sets used

2.1 GOSAT and GOSAT-2

The Greenhouse gases Observing SATellite (GOSAT; Kuze et al., 2009) was launched in January 2009 and is still in operation. The Thermal And Near infrared Sensor for carbon Observation (TANSO) on-board GOSAT consists of a Cloud and Aerosol Imager (TANSO-CAI) and a Fourier Transform Spectrometer (TANSO-FTS), which measures radiances in the NIR and SWIR spectral region with S and P polarisation and in the thermal infrared spectral region without polarisation with a spectral resolu-

tion of $0.2\,\mathrm{cm}^{-1}$. The FOCAL retrieval uses as main input calibrated GOSAT L1B V220.220 spectra from the three NIR/SWIR bands (around 0.76, 1.6 and $2.0\,\mu\mathrm{m}$) of TANSO FTS.

GOSAT-2 (Nakajima et al., 2017; Suto et al., 2020) was launched in October 2018 and comprises a similar instrumentation
as GOSAT. The GOSAT-2 FTS has the same spectral resolution but an extended spectral range for SIF and CO retrievals.

We use calibrated GOSAT-2 L1B NIR/SWIR data V101.101.

Both GOSAT and GOSAT-2 perform point measurements with a spatial resolution (footprint diameter) of about $10\,\mathrm{km}$. For both instruments, we use a tabulated instrumental line shape (ILS) with a kernel width of $15\,\mathrm{cm}^{-1}$. For GOSAT this has been generated by a theoretical formula parameterising a "real-world" FTS instrument (see e.g. formula 5.21 in Davis et al., 2001) ,
which depends on the maximum optical path difference (MOPD, $\pm 2.5\,\mathrm{cm}$ for GOSAT) and the size of the instantaneous field of view (IFOV, $15.8\,\mathrm{mrad}$ for GOSAT). The same formula has been used by Heymann et al. (2015). This ILS is symmetric and the same for S and P polarisation.

For GOSAT-2, we use a preliminary tabulated ILS provided by JAXA and generated on 16 January 2020, which is different for S and P polarisation and asymmetric, especially in the ~~SWIR-1~~ NIR band. Meanwhile, this ILS has been officially released
and is available via the NIES web site.

2.2 Reference Spectra and External Databases

For the retrieval several reference spectra and databases are used.

The solar spectrum used in the forward model is based on a high resolution solar transmittance spectrum (O'Dell et al., 2012) in combination with an ISS solar reference spectrum (Meftah et al., 2018). For the SIF retrieval we used a chlorophyll
fluorescence spectrum by Rascher et al. (2009), which has been scaled to $1.0\,\mathrm{mW/m^2/sr/nm}$ at $760\,\mathrm{nm}$.

We use tabulated cross sections at a $0.001\,\mathrm{cm}^{-1}$ sampling based on HITRAN2016 (Gordon et al., 2017) and the absorption cross section database ABSCO v5.0 (Benner et al., 2016; Devi et al., 2016) from the NASA (National Aeronautics and Space Administration) ACOS/OCO-2 project.

Surface elevation, surface roughness and surface type are derived 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) at a spatial resolution of $0.025°$. Meteorological information (pressure, temperature, water vapour profiles) is obtained from ECMWF (European Centre for Medium-range Weather Forecasts) ERA 5 model data (Hersbach et al., 2020), which are available every 1 hour on a $0.25°$ horizontal grid and on 137 altitude layers.

We use XCO_2 data from the CarbonTracker (CT) model CT2019 and CT-NRT v2020-1 (Jacobson et al., 2020a, b) and data
from the Total Carbon Column Observing Network (TCCON, see e.g. Wunch et al., 2011a) in the context of the bias correction reference database (see section 2.3). TCCON data are also used for validation (see section 5). Table 1 lists the TCCON stations which provided data for the present study.

XCO_2 a-priori profiles are derived using the 2018 version of the simple empirical CO_2 model SECM (Reuter et al., 2012). In the context of validation, we use the 2020 version of SECM. XCH_4 a-priori data are from the simple CH_4 climatological
model SC4C2018 developed and used by Schneising et al. (2019) and briefly described by Reuter et al. (2020).

For CO_2 we use the "synth" a-priori error covariance matrix described by Reuter et al. (2017b). For H_2O, we use the same error covariance matrix as Reuter et al. (2017b), but scaled by a factor of 5 to reduce the dependencies of the retrieval results on the a-priori. For CH_4, for convenience, we scale the CO_2 matrix to result in an XCH_4 uncertainty of 45 ppb, which is considered to be a reasonable estimate. Note that only the matrices are scaled, not the a-priori values.

2.3 The ~~"true"~~ reference database

Quality filtering and bias correction usually require the knowledge of a "true" (in this case XCO_2) value. For this, we do not simply use model data as truth, as one aim of XCO_2 products is to improve models. Another method is to take ground-based TCCON measurements as basis for a bias correction. However, although TCCON measurements are very accurate (estimated 1-σ precision is 0.4 ppm, see Wunch et al., 2010), they are only available at certain locations and are therefore more suited for validation.

Our choice is therefore to use a data base generated from a combination of TCCON measurements and CarbonTracker (CT) model data for a reference year (2018 for GOSAT, 2019 for GOSAT-2), which should on average reproduce large scale features correctly.

This database is produced in the following way: As a first step, we determine from the CT data global daily 3D maps close to 13:00 local time (i.e. GOSAT and GOSAT-2 equator crossing time). We reduce the altitude grid to five layers with the same dry-air sub-columns, i.e. the same amount of particles, and interpolate the data from the native CT horizontal resolution of $3° \times 2°$ to $0.5° \times 0.5°$. Then we determine from the TCCON data ~~daily~~ for each day mean values (XCO_2^{TCCON}) for 13 h $\pm$ 2 h local time. Next, we select collocated CT data and correct them for the TCCON averaging kernels, resulting in a TCCON corrected CT value at the TCCON location (XCO_2^{CT}). The application of the averaging kernels corrects for different vertical resolutions/sensitivities ~~.~~ (see e.g. Rodgers and Connor, 2003; Wunch et al., 2010). We look for contiguous regions where CT XCO_2 data differ by less than 0.75 ppm from ~~CT~~ the CT value at the TCCON location; these data are then used for the ~~"true" database.~~ reference database. The reference database therefore does not contain any TCCON data - it only contains CT data which were confirmed by TCCON, but individual values may differ by up to 1.5 ppm. The choice of the 0.75 ppm ranges is based on a trade-off between accuracy (agreement with TCCON) and spatial coverage of the database.

The result are daily maps containing CO_2 data for five vertical sub-layer altitudes. The spatial coverage is usually not global and varies from day to day. There are typically more data in the southern hemisphere during the second half of the year compared to the first half of the year (see Fig. 1). When comparing with GOSAT or GOSAT-2 measurement results, the "true" XCO_2 is then computed from the CO_2 layers of the ~~true~~ reference database, considering the retrieval's averaging kernels.

Specifically, we use here for GOSAT CT2019 data in combination with TCCON GGG2014 (see Tab. 1) for 2018. For GOSAT-2 we also use TCCON GGG2014 data, but need to rely on CT-NRT v2020-1 for 2019. Because the CT NRT data are not yet available for the whole year 2019, the GOSAT-2 ~~"true"~~ reference database does not cover the whole year; there are essentially no data after August 2019. This is a limiting factor for GOSAT-2, especially because this also means that data in the southern hemisphere are less present in the 2019 database.

2.4 GOSAT Level 2 Products

To assess the quality of the newly created GOSAT-FOCAL XCO_2 products, they have been compared with several other well-established GOSAT Level 2 data sets (see section 5). The GOSAT BESD v01.04 product from IUP (Heymann et al., 2015) is a near-real time product generated in the context of the Copernicus Atmospheric Monitoring Service (CAMS, https://atmosphere.copernicus.eu/ (last access: 30-July-2020)) project. It is available from 2014 onward. The GOSAT RemoTeC v2.3.8 product from SRON (Butz et al., 2011) and the full-physics GOSAT product from the University of Leicester v7.3 (Cogan et al., 2012) were generated in the context of the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/; last access: 30-July-2020) and cover the GOSAT time series from 2009 until end of 2019. The recently released NASA GOSAT ACOS v9r product (O'Dell et al., 2012, 2018; Kiel et al., 2019) is also available for the years 2009 to 2019. The operational GOSAT XCO_2 product v02.95 (bias corrected) from NIES (Yoshida et al., 2013) currently ends in August 2020. The BESD product contains only XCO_2 data over land, all other products are available for water and land surfaces.

3 Retrieval Algorithm

The retrieval is performed in three main steps: Pre-processing, processing and post-processing. These are described in the following sub-sections.

3.1 Pre-Processing

During pre-processing all required input data for the main processing step are collected. Furthermore, a first filtering of data is performed to reduce processing time.

The pre-processing procedure is largely based on the pre-processing as present in the BESD GOSAT product (Heymann et al., 2015). The sequence of pre-processing activities is as follows:

1. Extraction of measured spectra, geolocation and information on quality and measurement modes (e.g. gain, scan direction) from the GOSAT L1B product.

2. Estimation of instrument noise and cloud parameters.

3. Filtering for data quality, latitudes, solar zenith angle, signal-to-noise ratio and clouds (see Tab. 2 for settings).

4. Extraction of surface type, elevation and roughness derived from the surface database for each measurement.

5. Addition of corresponding meteorological information (pressure, temperature, dry-air column and water vapour profiles) for the time and place of the measurements. This includes a correction for surface elevation, i.e. model profiles are extended / cut according to the value from the surface database.

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6. Add a-priori gas profiles for each measurement (CO_2 from SECM, CH_4 from SC4C, H_2O from meteorology). For GOSAT-2, also a-priori profiles for CO and N_2O are added. The latter do not depend on geolocation; they are based on the tropical reference atmosphere from Anderson et al. (1986), scaled to column average values of XCO = 0.1 ppm and XN_2O = 330 ppb.

Because FOCAL is a fast algorithm and the number of GOSAT and GOSAT-2 measurements is much less than for OCO-2, we chose to set the pre-processing filters relatively relaxed and to apply the quality filtering mostly in the post-processing. As can be seen from Fig. 2 about two thirds of the measurements are filtered out during pre-processing.

3.1.1 Noise Estimate

Similar to Heymann et al. (2015) the spectral noise is initially assumed to be independent from wavenumber for each band. It is estimated from the standard deviation of the real part of the "dark" off-band signal (i.e. the first 500 spectral points in each band). In a later step (see Section 3.2.1) this noise will be modified to account for additional forward model errors and overall scaling.

3.1.2 Cloud Filter

The cloud filtering is based on two physical properties of clouds: clouds are (usually) bright and clouds are high (higher than the surface) so that little water vapour is above them. In the pre-processing these properties are described by two quantities: ~~cloud~~ effective albedo and water vapour ~~path.~~ filter. These are derived for each spectrum as described in Heymann et al. (2015). The ~~cloud~~ effective albedo for each band is estimated from the mean reflectance L within a spectral range outside the absorption. L is determined from the mean radiance I, the mean irradiance I_0 and the solar zenith angle α via:

$$L = \frac{\pi I}{I_0 \cos \alpha} \tag{1}$$

The specific wavenumber ranges and irradiance values used for filtering are given in Tab. 3.

The water vapour ~~path~~ filter is determined from a spectral region with strong water vapour absorption in the SWIR-3 band (see Tab. 3). ~~It is given by~~ This filter is defined as the ratio between the median radiance and the median of the estimated noise in this spectral range.

A ground pixel is assumed to be cloudy if either the ~~cloud~~ effective albedo in one of the bands or the water vapour ~~path~~ filter exceeds the thresholds given in Tab. 2.

3.2 Processing

The processing is based on the Fast atmOspheric traCe gAs retrievaL (FOCAL) algorithm which is described in detail in Reuter et al. (2017c). A first successful application of this algorithm to OCO-2 data is given in Reuter et al. (2017b). Therefore, we only summarise the main features of the algorithm here and point out the differences to the OCO-2 application.

FOCAL ~~appoximates~~ approximates modifications of the direct light path due to scattering in the atmosphere by a single scattering layer, which is characterised by its height (pressure level), its optical thickness and an Ångström parameter which

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describes the wavenumber dependence of scattering. The layer height is normalised to the surface pressure. Furthermore, Lambertian scattering on the surface is considered. For atmospheric scattering processes an isotropic phase function is assumed. With this approximation, the FOCAL forward model is essentially an analytical formula; it uses pre-calculated and tabulated cross sections such that calculations can be performed considerably fast. The inversion of the forward model is based on optimal estimation (Rodgers, 2000) and uses the Levenberg-Marquardt-Fletcher method (Fletcher, 1971) to minimise the cost function.

The OCO-2 retrieval of Reuter et al. (2017b, c) uses four fit windows in the NIR (near-infrared) and SWIR spectral range to derive the atmospheric parameters XCO_2, water vapour and SIF. In contrast to OCO-2, GOSAT and GOSAT-2 cover a wider spectral range and provide spectra in two polarisation directions referred to as S and P. Therefore, we treat in our retrieval both polarisation directions as independent spectra opposed to the average of both as usually used in other GOSAT retrievals (see e.g. Butz et al., 2011; Cogan et al., 2012; O'Dell et al., 2012). However, recently Kuze et al. (2020) presented a methane retrieval for GOSAT based on an algorithm from Kikuchi et al. (2016), which also makes use of both polarisation directions.

We use both polarisation corrections mainly for the following reasons:

- In principle, information is lost when averaging S and P spectra.

- In general, the sensitivity of the instruments and therefore the calibration of the measured spectra is different for S and P. For example, the measured ILS is given independently for S and P.

- S and P include different information on scattering, which can also be used in filtering and/or bias correction.

Furthermore, the FOCAL fitting windows (see Tab. 4) have been adapted to the specific GOSAT(-2) spectral bands such that in addition also other atmospheric constituents and parameters like HDO and (in the case of GOSAT-2) also CO total columns and possibly XN_2O can be retrieved. This results in six fitting windows for GOSAT and eight windows for GOSAT-2 for each polarisation. The retrieval is performed on a wavenumber axis.

Because of the large number of target gases and spectral bands the retrieval requires various state vector elements. These are listed together with the fit windows, from which they are determined, and their a-priori values and uncertainty ranges in Tab. 5 for GOSAT and GOSAT-2.

For GOSAT, the retrieval determines CO_2, CH_4 and H_2O on 5 layers with same number of air particles, from which then the column average values XCO_2, XCH_4 and XH_2O are calculated. Furthermore, solar induced fluorescence (SIF) is determined by scaling of a corresponding reference spectrum.

Instead of the HDO column, we fit a scaling factor for the relative abundance of HDO compared to H_2O, δD, which is defined as:

$$\delta D = \frac{R_{\mathrm{meas}}}{R_{\mathrm{VSMOW}}} - 1 \tag{2}$$

where R_{meas} is the ratio of the measured HDO and H_2O columns, R_{VSMOW} ($= 3.1152 \times 10^{-4}$) is the corresponding value for Vienna Standard Mean Ocean Water (VSMOW). δD is usually given in units of per-mill.

$\delta D = 0$‰ corresponds to HDO concentrations as in VSMOW, $\delta D = -1000$‰ to no HDO. We assume the same profile shape for HDO as for H_2O. For GOSAT-2, we also fit scaling factors to (fixed) CO and N_2O profiles.

As mentioned above, atmospheric scattering is considered in FOCAL by a single scattering layer, which is described by three parameters (height, optical depth and Ångström coefficient). As scattering is different for S and P polarised light, we fit two independent layers for S and P.

In addition, we determine in each fit window (independently for S and P) a polynomial background function describing the surface albedo. For this we use second order polynomials except for the small SIF windows (no. 1) where a linear function is sufficient.

The GOSAT data files only contain a fixed spectral axis. As e.g. described in Heymann et al. (2015), the spectral calibration of GOSAT changes especially at the begin of the mission with time. This change can be corrected by a spectral scaling factor. We determine this overall scaling factor by a spectral fit in the SIF window before the retrieval. So far, this spectral pre-fitting seems to be unnecessary for GOSAT-2. In the retrieval, we then additionally consider for both GOSAT and GOSAT-2 possible additional spectral shifts and squeezes in each fit window by corresponding state vector elements, but the influences of these spectral changes on the results is rather small.

3.2.1 Noise Model

The noise N derived from the off-band signal is only an estimate. It does not consider a possible wavenumber dependence of the noise within one spectral band. Furthermore, a potential error of the forward model needs to be considered. In the optimal estimation method this can be achieved by including the forward model error in the measurement error covariance. For this, we define a scaling factor s for the estimated noise and the quantity δF, which denotes the relative error of the forward model. The forward model error is proportional to the continuum radiance outside the absorption I, which is estimated from the 0.99 percentile of the measured radiance at the edge of each fit window. The quantities δF and s are determined using the approach described in (Reuter et al., 2017b), i.e. by running the retrieval for a representative subset of data and then fitting the function

$$RSR(NSR) = \sqrt{(s\,NSR)^2 + \delta F^2} \tag{3}$$

to binned values of the residual-to-signal ratio (RSR) as function of the noise-to-signal ratio (NSR). RSR is defined as the standard deviation of the retrieved spectral residual in each fit window divided by the continuum signal I; NSR is the standard deviation of the noise divided by I.

With the method described in Reuter et al. (2017c) it is also possible to define a 2σ-outlier limit based on NSR and RSR data, which will be used to filter out too noisy data during post-processing (see section 3.3). This is parameterised by a second order polynomial as a function of the uncorrected NSR

$$f_N(NSR) = a_0 + a_1\,NSR + a_2\,NSR^2 \tag{4}$$

which is added to the RSR function of Eq. (3). The coefficients a_i are determined via a fit. To avoid extrapolation, f_N is set to the edge values outside the fitting range.

In order to cover the varying signal over the year, we base the noise model fits on data from one day per month for one reference year. For GOSAT, we take from December 2017 to November 2018 (as there are only few GOSAT data available in December 2018). For GOSAT-2 we use data from February 2019 to December 2019. In the case of GOSAT-2 we further restrict the input data for the noise model parameter fit to data over land because some of the data over water show an unexpected behaviour (low RSR in case of large NSR), which needs further investigation. In this sense, the current GOSAT-2 noise model is considered to be preliminary and may need some refinement in the future.

~~Figs. ?? to ?? show~~

Fig. 4 shows as an example the noise model results for GOSAT and GOSAT-2 in the fit windows 2 ($O_2(A)$ band) and 6 (strong CO_2 absorption) for P polarisation. The orange line gives the fitted RSR function, the red line the outlier limit. The derived values from the noise model for all fitting windows / polarisations are given in Tab. 6 and 7 for GOSAT and GOSAT-2. The forward model errors δF are on average slightly larger for GOSAT-2 than for GOSAT. In the SWIR, values similar to OCO-2 are obtained, but in the NIR the OCO-2 δF is typically smaller (about 0.003). This indicates that for GOSAT and GOSAT-2 instrumental/calibration effects seem to impact the radiance errors more in the NIR than in the SWIR.

3.3 Post-Processing

The purpose of post-processing is to filter out invalid data and to perform a bias correction for the products. The current post-processing focuses on XCO_2. The post-processing is performed in several steps, namely:

1. Basic filtering based on physical knowledge.

2. Filtering out low quality data using parameters / limits determined using a random forest classifier.

3. Application of a bias correction using a random forest regressor.

4. Additional filtering out of data with too large bias correction.

These steps are described in the following subsections.

3.3.1 Basic filter

The basic filtering removes measurements where the retrieval does not converge or where the quality of the fit results is too low. We consider this to be the case if the χ^2 calculated over all fit windows is larger than 2 or if for at least one of the fit windows the RSR outlier limits (see section 3.2.1) are exceeded. Furthermore, we apply some initial filters for nonphysical values on the derived scattering parameters (i.e. layer height outside the atmosphere, Ångström coefficient not within [1,5]~~.~~). Note that all retrieved scattering parameters such as the Ångström exponent can be considered "effective" parameters as they have to account for not only cloud/aerosol scattering but also Rayleigh scattering (which has an Ångström coefficient of 4). Because Rayleigh scattering is always present and we filter out cloudy scenes, we usually get higher effective Ångström coefficients than those expected from clouds or aerosols only.

We also limit the maximum allowed optical depth of the scattering layer to 0.02 to filter out too thick clouds or aerosol amounts and use a maximum allowed XCO_2 ~~error~~ posteriori uncertainty of 2 ppm. As described by Reuter et al. (2017c), FOCAL simulates scattering only for an isotropic phase function. The prominent forward peak, usually existing for Mie scattering phase functions of cloud and aerosol particles does basically not modify the ~~lightpath~~light path. As FOCAL's optical depths of the scattering layer do not include this forward peak, these optical depths are much smaller than optical depths including a strong forward peak while having a similar influence on the light path modification (see discussion in the publication of Reuter et al. (2017c)). The maximum value of 0.02 for the layer optical depth should therefore not be interpreted as e.g. an aerosol optical depth.

The limits for the optical depth of the scattering layer and the XCO_2 error are somewhat arbitrary and actually result from visual inspection of the retrieval results. However, they are only intended as a first rough quality filter to facilitate later filter and bias correction methods, which will partly use the same parameters (see below). The detailed choice of these limits is therefore considered uncritical for the final results.

The above mentioned filter parameters and limits (see Tab. 8) are applied to both land and water surfaces and are the same for GOSAT and GOSAT-2, except for the RSR outlier limit which has been determined individually for each instrument. Figs. 2 and 3 show ~~exemplary~~ how many data points are typically filtered out in this step. The different performance of the RSR filters for both instruments indicates that the filtering for GOSAT-2 needs some further optimisation, which is planned for the next version of the products.

3.3.2 Random forest filter

In the next step, data are filtered out based on their expected XCO_2 bias i.e. the difference to a "true" XCO_2. Of course, this true XCO_2 value is normally not known. We therefore use the ~~"true"~~ XCO_2 reference database (as described in section 2.3) to train a random forest classifier (Pedregosa et al., 2011) to identify those variables which would remove – in combination with a corresponding random forest database – a pre-described percentage p of data based on their XCO_2 bias. This is done independently for data over land and water. Note that we are only interested here in the XCO_2 bias on top of an overall global bias as the latter will be handled via the bias correction.

This method is similar to the random forest filter used by Schneising et al. (2019) in the context of CH_4 and CO retrieval. Other approaches for data filtering used e.g. by Mandrake et al. (2013) and Reuter et al. (2017b) identify the best variables by minimisation of local XCO_2 variability in the retrieved products. However, all methods essentially serve the same purpose, i.e. to derive a reproducible filtering procedure which does not solely rely on expert knowledge.

We determine the list of relevant variables and the random forest database for the filtering in the following way: We use the (uncorrected) results of the retrieval for the reference and apply the basic filtering as described in section 3.3.1. Then, the subset of these data is selected which has a corresponding "true" value in the reference database. For these data we determine the XCO_2 bias (measurement - reference XCO_2) and subtract the ~~monthly global median~~global median for land and water of this bias. We then sort the data according to this bias and flag those p percent of data with the highest absolute bias values as "bad".

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For GOSAT, this results in a total number of 54317 data points over land and 109414 over water. These numbers are smaller for GOSAT-2 (land: 10625, water: 40459). The random forest classifier is then trained by using randomly 90% of these data as input. The training is done in two iterations: First, with a complete set of possible input variables ("features") and output variables ("estimators"); then, using only a reduced set consisting of the 10 best features/estimators, i.e. those with highest random forest score (relevance) of the first run. This relevance is a quantity which describes the relative importance of each feature for the filtering. Relevances are normalised such that the sum of all relevances is 1. The random forest classifier then decides for each measurement based on these 10 variables if it is filtered out or not.

The initial list of possible features/estimators includes essentially all quantities available after the retrieval, including viewing angles, surface properties and continuum signal for each fit window. Furthermore, the retrieved values of the state vector elements and their errors are included in this list as well as averaging kernels for the profiles. We explicitly exclude the geolocation of the measurement (latitude, longitude) and the retrieved values (but not the errors) for the data products we are interested in, i.e. the gases and SIF. This is to avoid e.g. the filtering out of certain geographical regions or removing all points with high XCO_2 values.

Note that in glint mode over ocean, the inclusion of information about the viewing geometry as possible features bears the risk that the random forest procedure may infer the geolocation from a combination of these.

However, we include as possible filter variable the gradient of the retrieved CO_2 profile (i.e. the difference between the two lowermost layers) as this has shown to be a suitable quantity.

The original number of candidate variables presented to the random forest classifier is quite high (193 for GOSAT and 246 for GOSAT-2) as can be seen from Figs. 5 and 6 (top left plots), but there are only few with a high relevance.

The ten best variables selected partly differ for land and water surface (as shown in the middle and left top panels), but they usually comprise scattering parameters, polynomial coefficients, spectral corrections and some XCO_2 related parameters.

The other 10% of the input data are used to test the performance of the classifier. The results from this test and other cross-validation activities indicate, that the random forest classification is – depending on surface – only accurate in about two thirds of the cases. This accuracy is defined as the fraction of correctly classified samples. This means that the filtering also removes possibly valid data points and does not remove all possibly bad ones. However, we do not expect a perfect classification, because it is not possible to describe all inter-dependencies via the set of input features. Note that the performance of the filter is similar for both the training and the test data sets. This indicates that there are no problems with over-fitting.

To obtain a high quality of the remaining XCO_2 data, we therefore need to filter out quite a large percentage of data (and perform an additional filtering at a later time, see below). For future data products further investigations are planned to improve the performance of the classifier, e.g. by providing additional features from combination of existing ones (like the already used CO_2 gradient). The percentage p of data to be filtered out is usually a trade-off between data quality and remaining amount of data. In the present case a 50% limit has been selected. Actually, as can be seen from Figs. 2 and 3, the relative amount of data filtered out via the random forest classifier is not exactly 50% of the data remaining after the previous filters.

3.3.3 Bias correction and filtering

~~use for OCO-2~~ XCO$_2$ retrieval methods usually require a bias correction ~~based on the "small area approximation", which assumes that the variation of~~ to be applied to the data. This correction is often based on multi-linear regressions using parameters identified from correlation analyses of differences to an assumed "true" XCO$_2$ ~~within a small area is small. This~~ data set. Different data products use different methods to define this "truth". In many cases, ground based TCCON measurements are taken as reference for the "true" XCO$_2$, like in the GOSAT BESD product (Heymann et al., 2015), the SRON products (Guerlet et al., 2013), the product from the University of Leicester (Cogan et al., 2012) and also the operational GOSAT product from NIES (Inoue et al., 2016). The bias correction of the NASA ACOS OCO-2 product is quite complex (O'Dell et al., 2018; Kiel et al., 2019); it uses as reference a modification of the "Southern Hemisphere Approximation" introduced by Wunch et al. (2011b). The ACOS products takes multi-model mean data as reference and derives corrections from data in the southern hemisphere below 20°S where CO$_2$ is assumed to be quite uniform on small areas. A similar "small area approximation" is also used by Reuter et al. (2017c) to correct FOCAL OCO-2 data. This correction method is not possible for GOSAT and GOSAT-2 data because of their sparse sampling. We therefore follow a different approach here.

For the bias correction we use as input the same data set as for the random forest filter, but with this random forest filter applied. 50% of the resulting data set is then used to train a random forest regressor (see also Schneising et al., 2019), which aims to minimise the "true" XCO$_2$ bias(, i.e. the difference to the reference database value without global median subtracted)~~)~~, as function of the specified features. To create the bias correction database and the corresponding list of best features we again run the training twice, first with the full list (the same as for the filter) and then with the top ten features. Again, we use different corrections for land and water. The resulting parameters and their performance are shown in the bottom panels of Figs. 5 and 6. The bias correction selects similar best features as the filter, but not exactly the same quantities in the same sequence.

~~During application of the bias correction , the random forest regressor estimates the bias based on the values of the input variables . This bias is then subtracted from the retrieved value. Application~~ The actual number of features/variables to be used for both filtering and bias correction is a trade-off between many variables (explaining all relations with a risk for over-fitting and high computational effort) and few variables (no over-fitting, but maybe missing some relations). Considering ten features for the bias correction is more than other algorithms typically use, but this is appropriate in our case because we take into account the different relevance of these parameters, which drops off rapidly within the first ten variables (see top panels of Figs. 5 and 6).

The validity of this choice is confirmed by the application of the bias correction to the training data set and the other 50% of the input data, which shows a comparable reduction of the XCO$_2$ scatter~~, which~~. This is an indication for a good performance (e.g. no over-fitting) of the regressor.

During application of the bias correction, the random forest regressor estimates the XCO$_2$ bias based on the values of the input variables. This bias is then subtracted from the retrieved value.

Currently, there is only a bias correction for XCO$_2$, but in principle this method is applicable also to other quantities depending on the availability of a corresponding ~~"true"~~ reference database.

After the bias correction there are still a few outliers left in the XCO$_2$ data. These are filtered out by an additional filter on the ~~derived~~ XCO$_2$ bias derived via the random forest classifier. The limits for this filter are the global median bias for test data

set $\pm 2\,\mathrm{ppm}$. the median bias is different for land and water surfaces and also for GOSAT and GOSAT-2. The actual limits are given in Tab. 9. The value $2\,\mathrm{ppm}$ is estimated from visual inspection of the data. Figs. 2 and 3 show that typically less than 1–2% of the remaining data (less than 0.1% of all) are affected by this last filter.

The spatial variability of the finally derived bias correction (see Fig. 7) is typically below $1\,\mathrm{ppm}$, but as mentioned above there is a systematic difference between land and water data of about of $1-1.5\,\mathrm{ppm}$ (see Tab. 9).

4 Results

The FOCAL retrieval has been applied to all GOSAT and GOSAT-2 measurements until end of 2019. On average, FOCAL needs $22\,\mathrm{s}$ with 6 iterations for the processing of one GOSAT ground pixel. For GOSAT-2 numbers are slightly larger ($28\,\mathrm{s}$/7 iterations) because of the additional fit windows and state vector elements. All performance values are given for a single core of an Intel Xeon E5-2667v3 CPU ($3.2\,\mathrm{GHz}$). These numbers are actually about one magnitude larger than the ones given in Reuter et al. (2017b, c) for the FOCAL application to OCO-2. This is because we use for GOSAT(-2) separate S and P polarisation spectra and more retrieved variables, which requires more and larger fit windows. For each of these fit windows and parameters, weighting functions have to be calculated, which involves a convolution with the ILS. This convolution is the most time consuming part of the FOCAL retrieval. This is even more relevant for GOSAT(-2), because the FTS ILS is in principle sinc-shaped, i.e. it has a sharp peak in the centre but wide wings, which requires a large kernel width (in our case $15\,\mathrm{cm}^{-1}$ for the convolution.

Figs. ?? to ??

The left plots of Figs. 8 and 9 show examples for measured and fitted nadir mode radiance spectra for GOSAT and GOSAT-2 over land in the different fitting windows for P polarisation. Since the difference between measured and modelled spectra is small and thus hard to see, we show in Figs. ?? to ?? these figures on the right side the corresponding residuals and the estimated noise. The results for S polarisation look similar and are therefore not shown here. The residuals are on the order of magnitude of the noise, which is slightly higher for P polarisation than for S polarisation. Some small spectral structures are visible in the residuals, they appear more clearly in the smoothed residuals (convoluted with a 21 pixel boxcar), e.g. for GOSAT and GOSAT-2 in the $O_2(A)$ band (window 2), and some broadband oscillations in window 4 and 5 for GOSAT-2. These features are present in both S and P polarisations and occur also in other measurements, so they seem systematic. A reduction of these features could possibly further improve future products.

In Fig. 10 some statistical information about the GOSAT-FOCAL data products is given. A time series for the number of valid data is given in the top plot. In the recent years, about 5–6% of the available measurements could be transferred to valid XCO_2 data. The number of valid data points increases from 2009 to 2019. This is mainly due to an increase in the data over water, which is most likely related to optimisations in GOSAT operations (better use of glint geometry) over water. As expected, the mean global XCO_2 shown in the middle plot increases with time. Global mean values over water are typically slightly higher than over land; this is most likely a spatial sampling issue. The observed XCO_2 variability (standard deviation, bottom plot) is larger over land which . Part of this variability is attributed to influences of surface elevation and to different scattering pathways

between the land and water measurements. For GOSAT-2, only retrieved data from 2019 are available so far. The total amount of available measurements is about 2.8 million, compared to about 3.5 million GOSAT measurements in 2019. Only about 3% of the GOSAT-2 data remain after all filtering / post-processing, which is roughly half of the corresponding number for GOSAT (but similar to the first year of GOSAT). As can be seen from Fig. 3 more GOSAT-2 data are filtered out due to failed or bad convergence and by the RSR outlier limits than for GOSAT (Fig. 2). Future improvements of the GOSAT-2 calibration or the noise model ~~could possibly~~ are considered to help here.

For further analyses, we have generated monthly maps on a $5° \times 5°$ grid. Example plots for the months April and August 2019 (begin/end of the growing season) are shown in Fig. 11 for GOSAT and in Fig. 12 for GOSAT-2. The data are not filtered for low amounts of input data in the grid points, which ~~may explain~~ explains some individual outliers in the plots. Overall, the spatial patterns observed by GOSAT and GOSAT-2 look reasonable. The north–south gradient in XCO_2 is visible with different sign in April and August for both instruments. The spatial coverage of the GOSAT-2 data is lower than for GOSAT, because more data are filtered out (see above). This ~~seems to affect~~ affects especially regions like the northern part of Africa.

5   Verification and Validation

For the verification and validation of the GOSAT and GOSAT-2 FOCAL products we perform a comparison with various reference data sets (see section 2), namely:

- The GOSAT BESD v01.04 product from IUP (referred to as "BESD" later).
- The GOSAT ACOS v9r product from NASA (referred to as "ACOS" later).
- The GOSAT UoL_FP v7.3 product from the University of Leicester (referred to as "UoL" later).
- The GOSAT RemoTeC v2.3.8 product from SRON (referred to as "SRON" later).
- The GOSAT operational product v02.95 (bias corrected) from NIES (referred to as "NIES" later).
- Collocated TCCON GGG2014 data (referred to as "TCCON" later).

For the comparisons, all data have been adjusted using the same a-priori (SECM2020).

Since all GOSAT products use different retrieval and filter methods, they do not contain the same number of data (see Fig. 13). Currently, the NASA ACOS product has the largest number of valid data points, followed by the new GOSAT-FOCAL product with about 20% less data.

5.1   Direct comparisons

There are enough common measurement points included in the different GOSAT products to perform a direct comparison. Figure 14 shows ~~exemplary~~ as an example a comparison between the GOSAT-FOCAL data for the year 2018 with the corresponding ACOS, BESD, SRON, NIES and UoL products. For each plot we only use data where both data sets have a valid

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XCO_2 value. For these data we performed a linear regression using the Orthogonal Distance Regression (ODR) method (see e.g. Boggs et al., 1987). Unlike common linear regression, ODR considers uncertainties for both axes (data sets) by minimising the orthogonal distances between the model curve and the data points. The ODR results are shown by the red line and its label. Number of collocations and median/mean and standard deviations of the differences are given in the titles.

Overall, the data scatter around the 1:1 line in a similar way for all comparisons. ODR slopes vary between the data sets from 0.84 (for FOCAL vs. ACOS) up to 1.08 (for FOCAL vs. BESD). Most collocations are available for the ACOS data set because this has the largest number of valid data. Mean and median differences are quite similar and reach from -0.17 ppm (comparison to BESD) to 0.67 ppm (comparison with UoL). The scatter (standard deviation of the differences) reaches from 1.4 ppm (ACOS, NIES) to 1.8 ppm (BESD).

5.2 TCCON comparisons

The TCCON network provides high-quality XCO_2 (and other) data which are currently considered to be the main reference for greenhouse gas data obtained from satellite measurements. Therefore we compared the different GOSAT data sets with collocated TCCON measurements from 2009 to the end of 2018. BESD data are not included, because they do not cover the complete time interval. Collocation criteria are:

– Maximum time difference of 2 h.

– Maximum spatial distance of satellite measurement from TCCON station 500 km.

– Maximum surface elevation difference between satellite measurement and TCCON station 250 m.

In addition to these criteria we also consider in the validation only stations / TCCON data sets, which have at least 50 collocations for all algorithms. This improves the comparability of regional and seasonal biases. As a consequence, not all stations listed in Tab. 1 contribute to the validation.

The comparison procedure is the same as used by Reuter et al. (2020) and described by Reuter et al. (2019b). In summary, for each TCCON site, the time series of satellite minus TCCON differences are computed under consideration of the averaging kernels, i.e. different vertical sensitivities. The resulting time series are fitted with a trend model, which includes an offset term, a slope term, and a sine term for seasonal fluctuations. The offset term is considered the station bias and the station scatter is computed from the standard deviation of the fit residual. Results for the GOSAT time series at the TCCON stations are shown in Fig. ~~??~~15. Overall, the temporal variations of XCO_2 are well reproduced by all data.

Figure ~~??~~ 16 shows as a summary of the GOSAT TCCON comparisons the derived bias and scatter for the different stations and products. The new GOSAT-FOCAL product compares well with the other data sets. Its differences to TCCON have a station to station bias (the standard deviation of the station bias) of 0.56 ppm and a mean scatter (RMS scatter per station) of 1.89 ppm. The seasonal component of the bias has a station to station average standard deviation of 0.37 ppm. Overall, the ACOS product performs best in this comparison.

Note that the biases shown in Fig. ~~??~~ 16 correspond essentially to a bias anomaly since a ~~global bias~~ the mean bias over all stations was removed from all products. ~~Therefore~~ This is because for most applications this mean bias is not relevant since most

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information is contained in gradients. Subtracting a mean bias also facilitates a comparison of different bias patterns between the algorithms. The subtracted mean station bias is actually small; for GOSAT it varies between 0.17 ppm (for ACOS) and 0.64 ppm (for NIES). Because of the subtracted mean bias different signs of biases for different products could be coincidental. However, the biases of FOCAL and ACOS are consistent with the biases found by Reuter et al. (2020).

500   In Figs. 17 and 18 we show results from a preliminary comparison of the new GOSAT-2 FOCAL data with TCCON. These results are considered less reliable, because they are based on a data set which covers less than a year. There are sufficient collocations for only seven TCCON stations, and some of them comprise only a few months of data, which limits the fit of our trend model. The mean scatter of the GOSAT-2 data is 1.86 ppm and therefore similar as the one for GOSAT. The derived station-to-station bias for GOSAT-2 FOCAL is 1.14 ppm. This high value is mainly due to the biases derived for the

505   stations Orleans and Reunion Island (where only few data are available) and the station Pasadena, which also showed larger discrepancies to the GOSAT products (see Fig. 16). We are confident that the station-to-station bias will improve when more and improved GOSAT-2 data will be available.

Via the TCCON comparison it is also possible to validate the reported precision of the FOCAL data products (i.e. the specified XCO_2 error). The basic idea is to estimate the "true" precision from the variability of the XCO_2 bias relative to

510   trend-corrected, collocated TCCON data. For this purpose, we define 20 bins with increasing reported XCO_2 uncertainty and compute the corresponding true precision from the scatter relative to TCCON (i.e., the fit residual mentioned above).

The corresponding scatter plot is shown in Fig. 19. We use the fitted linear curve to correct the reported uncertainty of the GOSAT-FOCAL data. After the correction, all data scatter around the 1:1 line (dashed).

A similar correction will be performed for the GOSAT-2 FOCAL product as soon as sufficient data (GOSAT-2 as well as

515   TCCON) are available, which is currently not yet the case.

5.3 Time series

To investigate the temporal behaviour of the FOCAL XCO_2 data sets, we performed comparisons based on monthly data from 2009 to 2019, which were spatially gridded to $5° \times 5°$ (examples are shown in Figs. 11 and 12). Similar data sets have been generated for the SRON, UoL, ACOS and NIES GOSAT products. We also produced a corresponding gridded GOSAT-BESD

520   data set; since these are near-real-time (NRT) data only, there are no GOSAT BESD data before 2014 available (when the NRT processing started). GOSAT-2 data start in February 2019.

We then selected for each combination of GOSAT-FOCAL XCO_2 and a correlative data set grid points where the standard error of the mean is less than 1.6 ppm (as a basic quality filter, similar as done by Reuter et al., 2020). These data were then averaged over different latitudinal ranges, namely:

525   – Global (90°S – 90°N)

– Northern hemisphere (25°N – 90°N)

– Tropics (25°S – 25°N)

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– Southern hemisphere ($25°$S – $90°$S)

Figure 20 shows the results of these comparisons. The left plots display time series of the different data sets, the right plots
the difference between the GOSAT-FOCAL XCO_2 and the reference data. All data products reproduce the overall increase
of XCO_2 with time as well as the seasonal variations. On average, FOCAL data are typically about 0.5 ppm higher than the
other data sets (except for BESD). This ~~is most likely~~ related to the choice of the "true" XCO_2 for the bias correction. There
are long-term changes in the order of 1 ppm over the complete time series, which differ for each data set. For example, the
GOSAT-FOCAL data show in the tropics relative to SRON a higher value at the start of the time series, but both data sets
agree at the end. On the other hand, the average difference to the UoL data in the northern hemisphere is negative during the
first years, but increases to an almost constant small positive offset below about 0.5 ppm. There is not much difference in the
temporal behaviour between the GOSAT-FOCAL and the ACOS and NIES time series. The seasonal shapes also differ slightly
with amplitudes of about 0.5 ppm with somewhat larger differences in the southern hemisphere where seasonal variations are
generally smaller.

Overall, the agreement within the GOSAT data sets is broadly consistent with the systematic regional and seasonal biases
derived from the TCCON validation, especially considering that all gridded data sets are based on a different spatial and
temporal sampling. Also, the FOCAL products for GOSAT and GOSAT-2 seem to agree quite well, but more GOSAT-2 data
is needed to confirm this.

6 Conclusions

Based on the FOCAL retrieval method a new XCO_2 data set for GOSAT and a first XCO_2 data set for GOSAT-2 have been generated, making use of both measured polarisation directions. The GOSAT-FOCAL data set compares well with corresponding
data from other currently available GOSAT retrieval algorithms, i.e. the RemoTec product from SRON, the UoL FP product,
the NASA ACOS product, the NIES product and the BESD product from IUP. All data sets use different filtering and bias correction schemes and therefore comprise also a different number and sampling of data. The GOSAT-FOCAL product performs
well in this context and has almost as many valid data as the ACOS product. Based on gridded data, differences in long-term
variations of all data sets in the order of 1 ppm per decade are observed. Also, seasonal variations differ by about 0.5 ppm.

Comparisons with ground-based TCCON data reveal for the GOSAT-FOCAL product an overall station to station bias of
0.56 ppm and a mean scatter of 1.89 ppm. These values are comparable to and in some cases even better than those of the
already existing GOSAT products of which some have less valid data.

The first GOSAT-2 results using the FOCAL method are also quite promising, but further investigations, longer time series
and more correlative data sets are required for a quantitative assessment of the GOSAT-2-FOCAL data quality.

Overall, the FOCAL method has proven to be computationally fast and to produce XCO_2 results with similar accuracy
as other, typically more time consuming, retrieval algorithms. This is the case not only when applied to OCO-2 but also for
GOSAT and GOSAT-2. FOCAL is therefore considered to be a good candidate algorithm for future satellite sensors producing
large amounts of data, like the forthcoming European anthropogenic CO_2 Monitoring (CO2M) mission.

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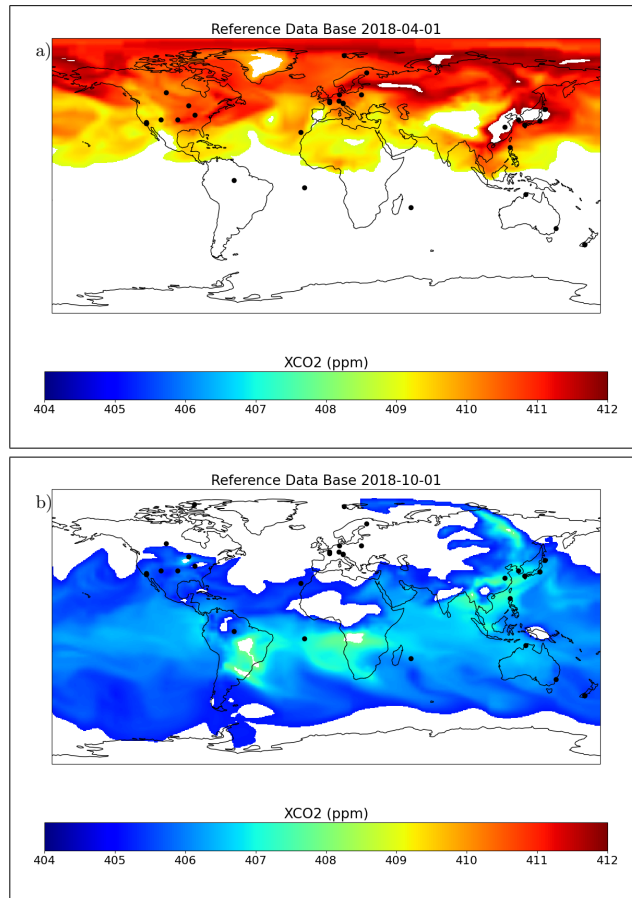
Figure 1. XCO_2 from the GOSAT-FOCAL reference database. The black markers show locations of TCCON stations. a) 2018-04-01. b) 2018-10-01.

~~GOSAT noise model (S polarisation).~~
~~GOSAT noise model (P polarisation).~~

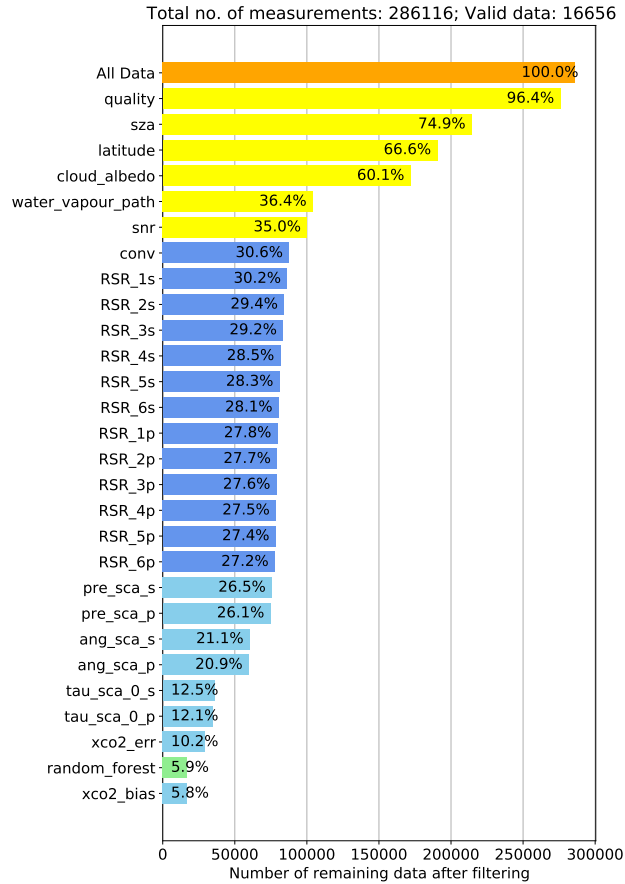Total no. of measurements: 286116; Valid data: 16656

Figure 2. Example for GOSAT data filtering during the different processing steps (April 2019). Filters are listed in sequential order from top to bottom on the vertical axis. Numbers in the horizontal bars denote the percentage of remaining data after this filter was applied. Orange: Total number of measurements before filtering. Yellow: Pre-processing filters. Blue: Step 1 post-processing filters (convergence and noise). Green: Random forest post-processing filter. Light blue: Additional post-processing filters.
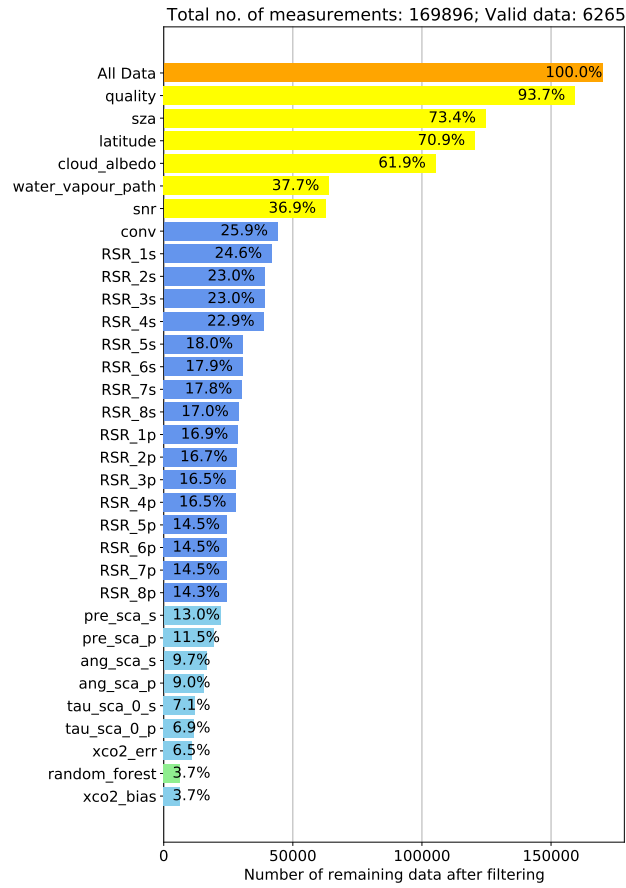
Figure 3. Same as Fig. 2, but for GOSAT-2.
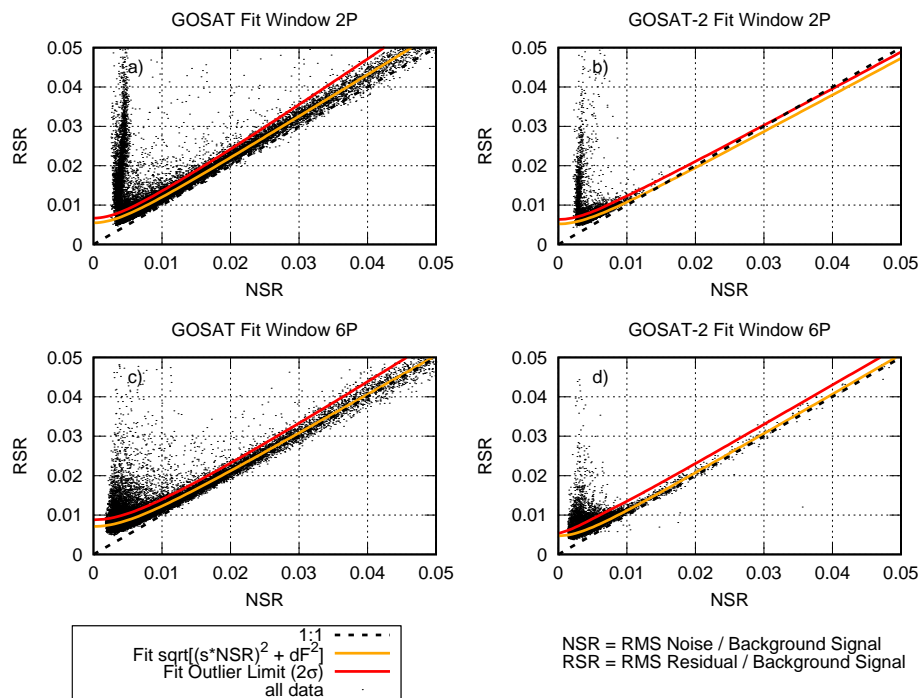
Figure 4. ~~GOSAT-2~~ Example results from the noise model~~(S polarisation~~. a) GOSAT fit window 2P. b) GOSAT 2 fit window 2P. c) GOSAT fit window 6P. d) GOSAT 2 fit window 6P.

~~GOSAT-2 noise model (P polarisation).~~
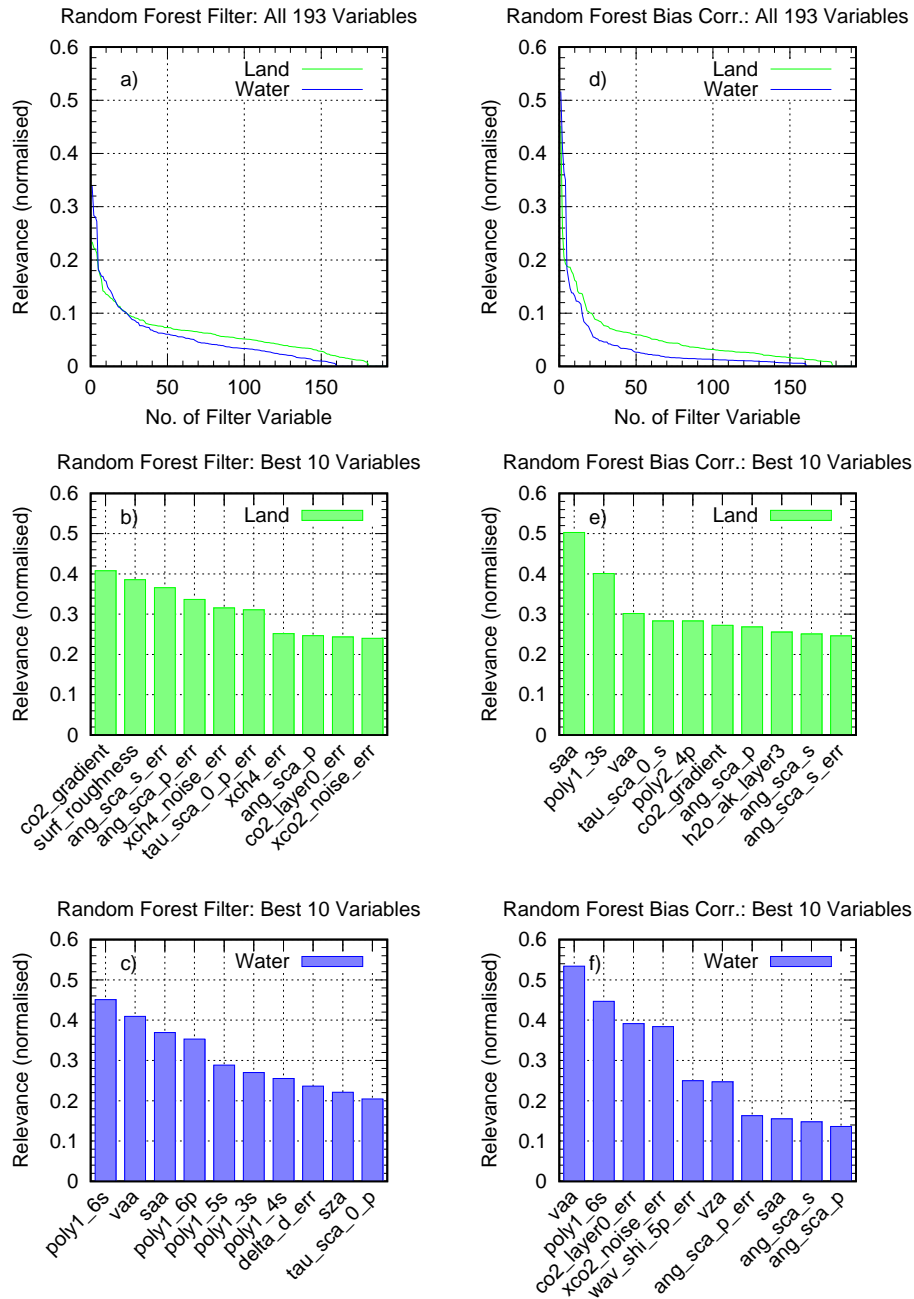
Figure 5. Random forest results for GOSAT. Left (a–c): Results from random forest filter. Right (d–f): Results from random forest bias correction. Top: Normalised relevance (score) of all filter variables. Middle/bottom: Selected variables and their relevance for land/water surface.
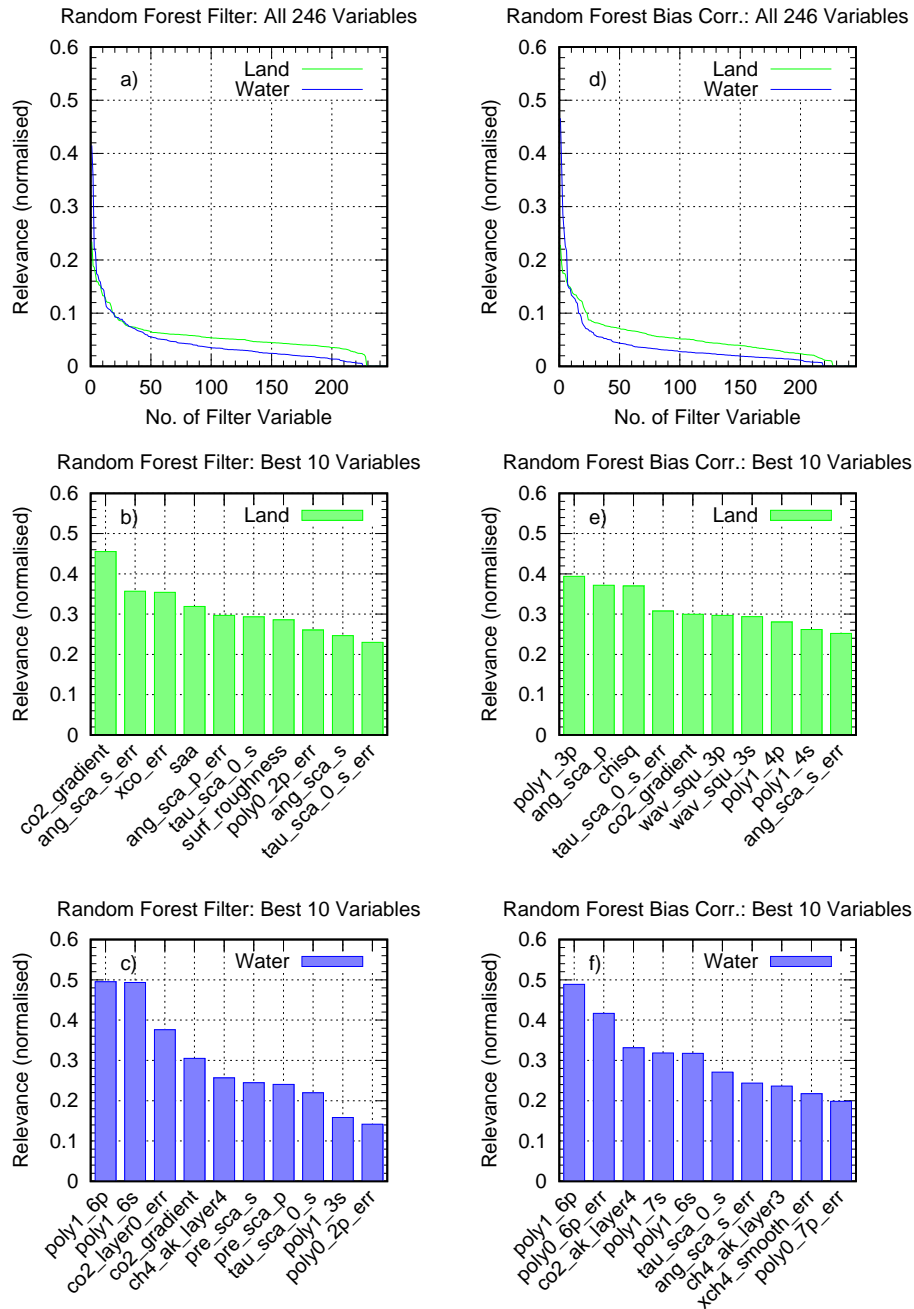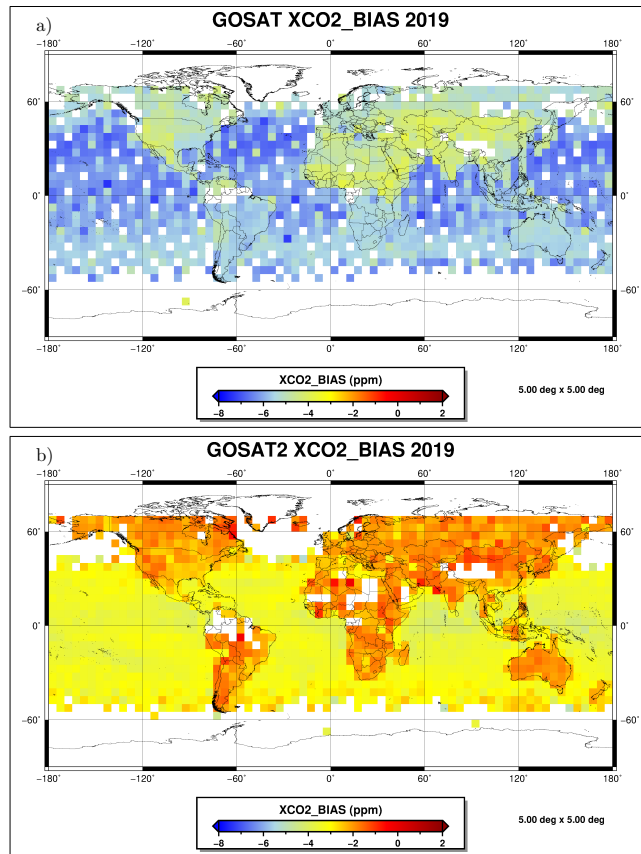
Figure 6. As Fig. 5, but for GOSAT-2.

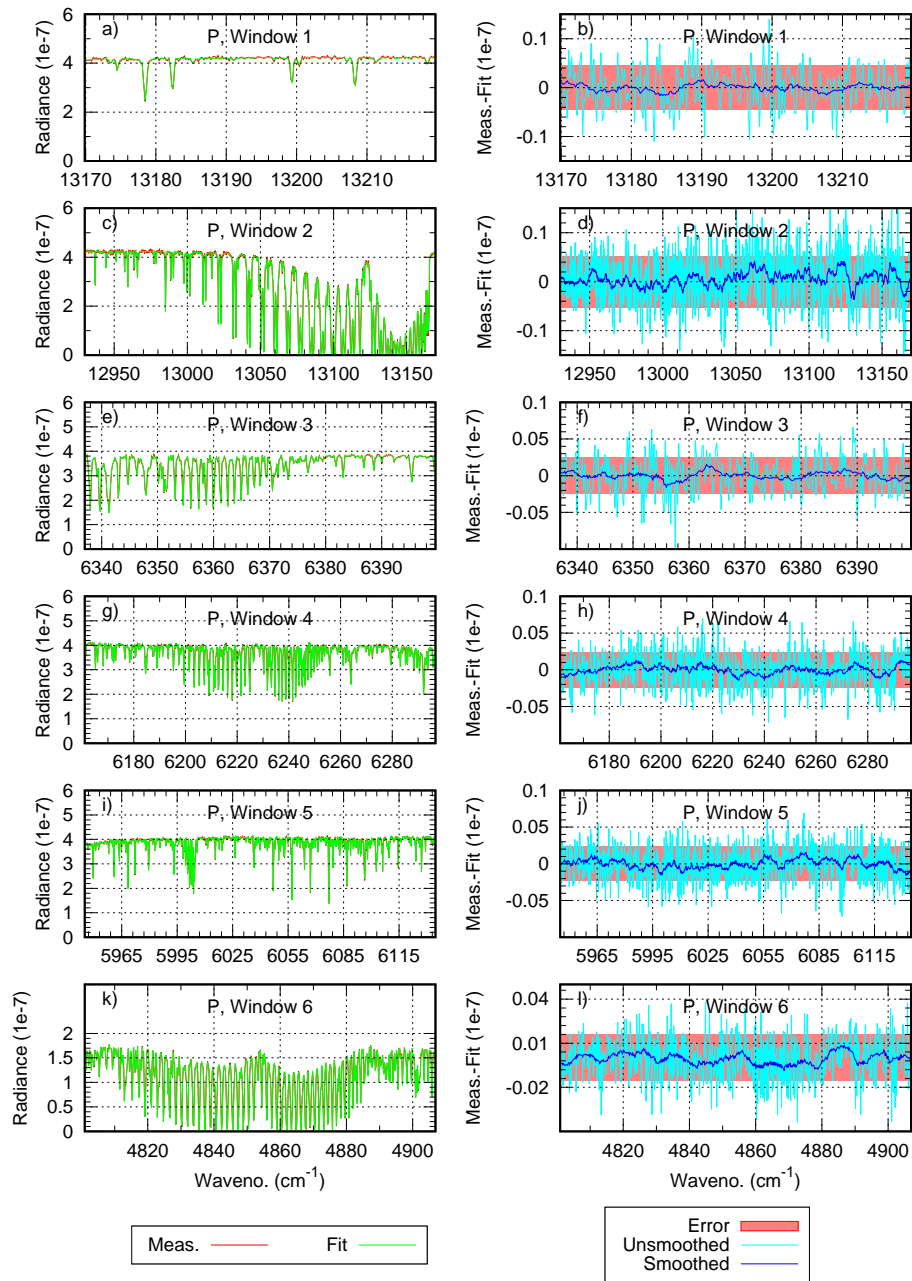**Figure 7.** Gridded GOSAT (a) and GOSAT-2 (b) XCO_2 bias correction for 2019.

Figure 8. Example for a single GOSAT measurement (S̶ P polarisation): Left: Measured (red) and retrieved (green) spectra in the different fit windows; because of the good agreement the red curve is essentially barely visible below the green curve. Right: Corresponding residuals (measurement - fit). Light Blue: Unsmoothed. Blue: Smoothed with a boxcar of width 21 spectral pixels (= $4.2\,\mathrm{cm}^{-1}$). Red: Estimated noise error range. Radiance unit is $\mathrm{W/cm}^2/\mathrm{cm}^{-1}/\mathrm{sr}$.
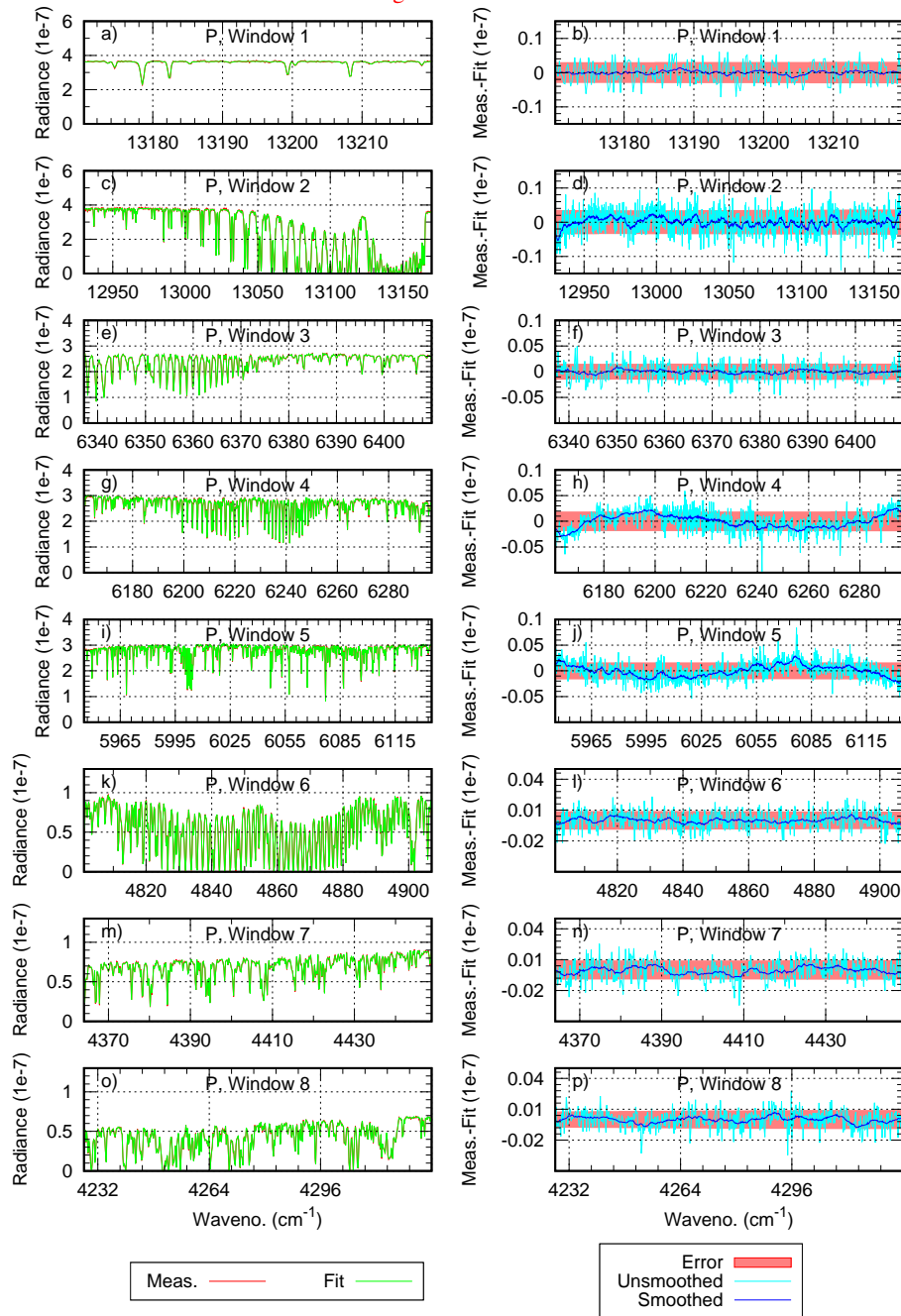
40

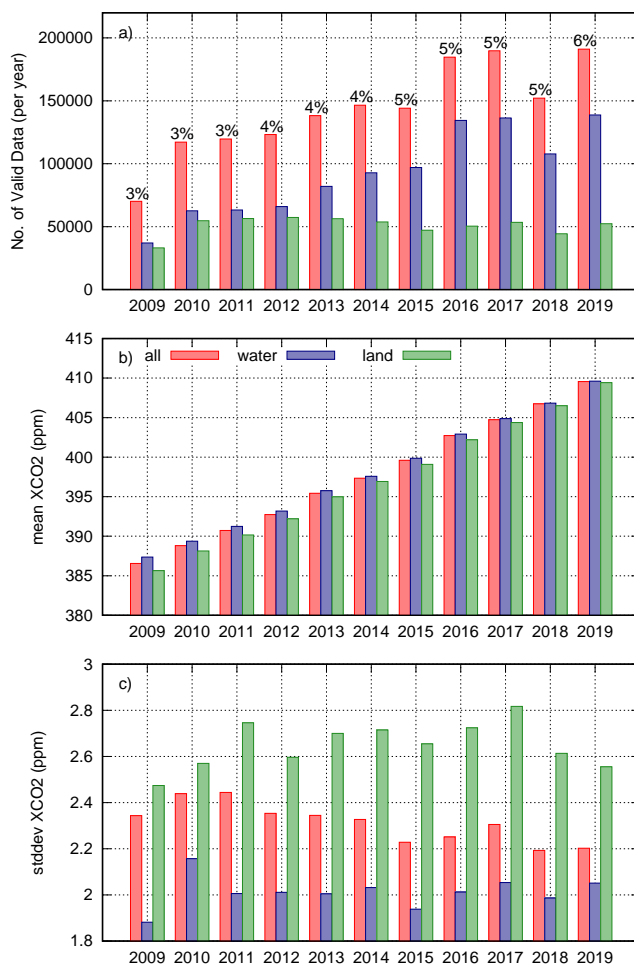**Figure 9.** Same as Fig. ~~??~~ 8 but for GOSAT-2.

Figure 10. Statistics for valid GOSAT measurements (after pre- and post-processing filtering) for each year. Blue: Measurements over water. Green: Measurements over land. Red: All data. a) Number of valid measurements, incl. percentage of all originally available measurements. b) Global mean XCO_2. c) Corresponding standard deviation.
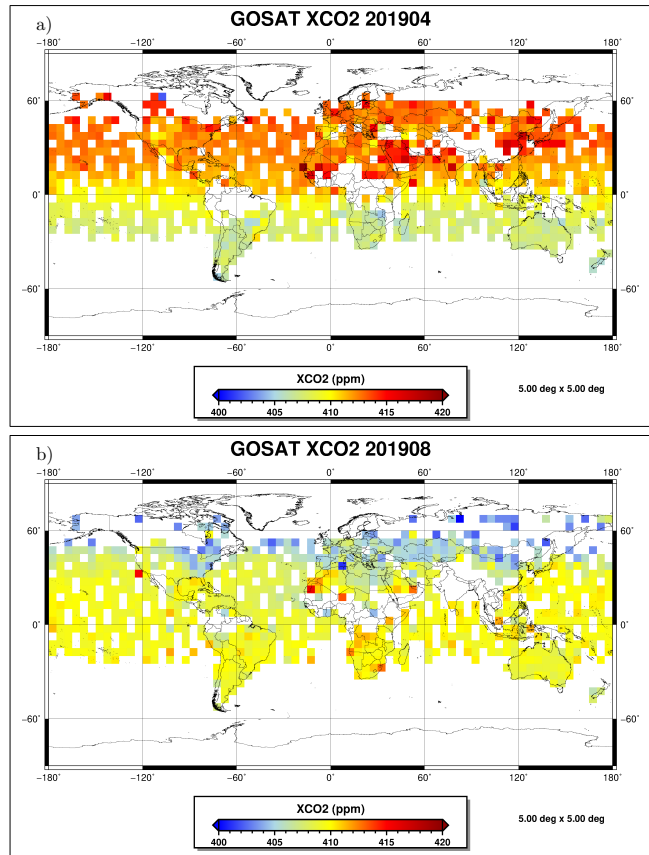
Figure 11. Example for gridded GOSAT XCO_2 data. a) April 2019. b) August 2019.
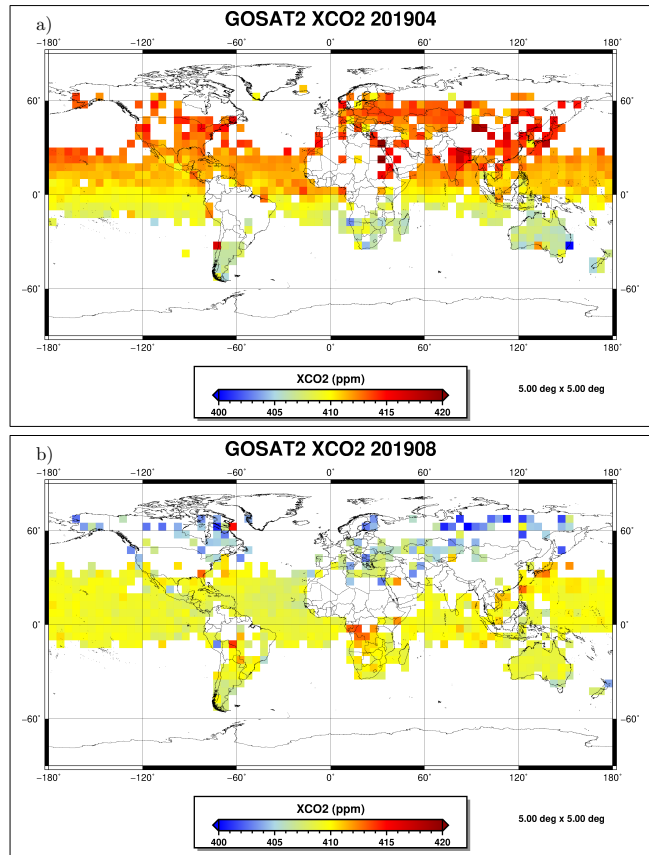
Figure 12. Example for gridded GOSAT-2 XCO_2 data. a) April 2019. b) August 2019.
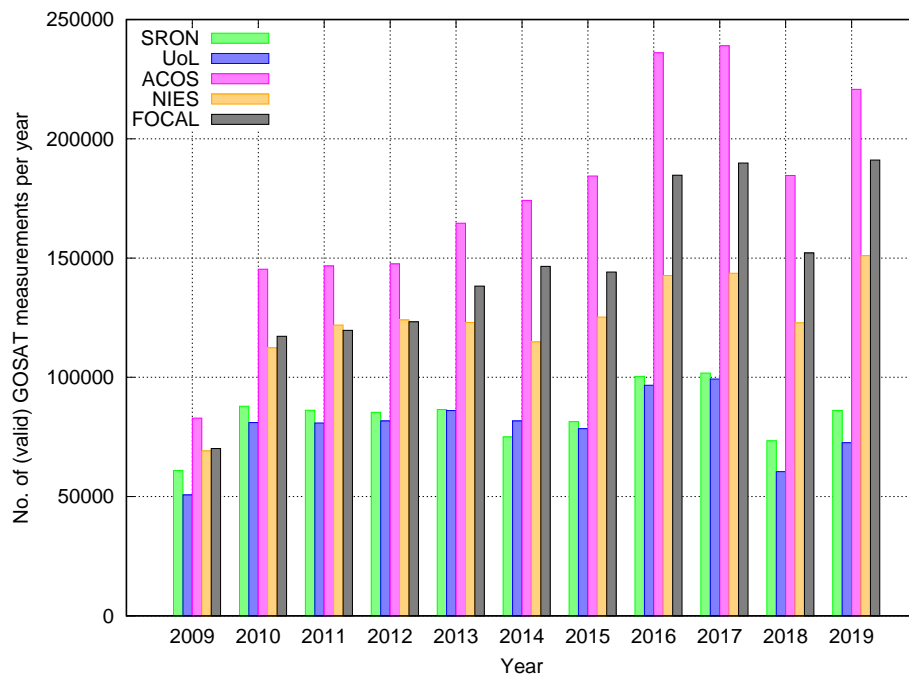
Figure 13. Number of valid XCO_2 data points in the different GOSAT products from 2009 to 2019.
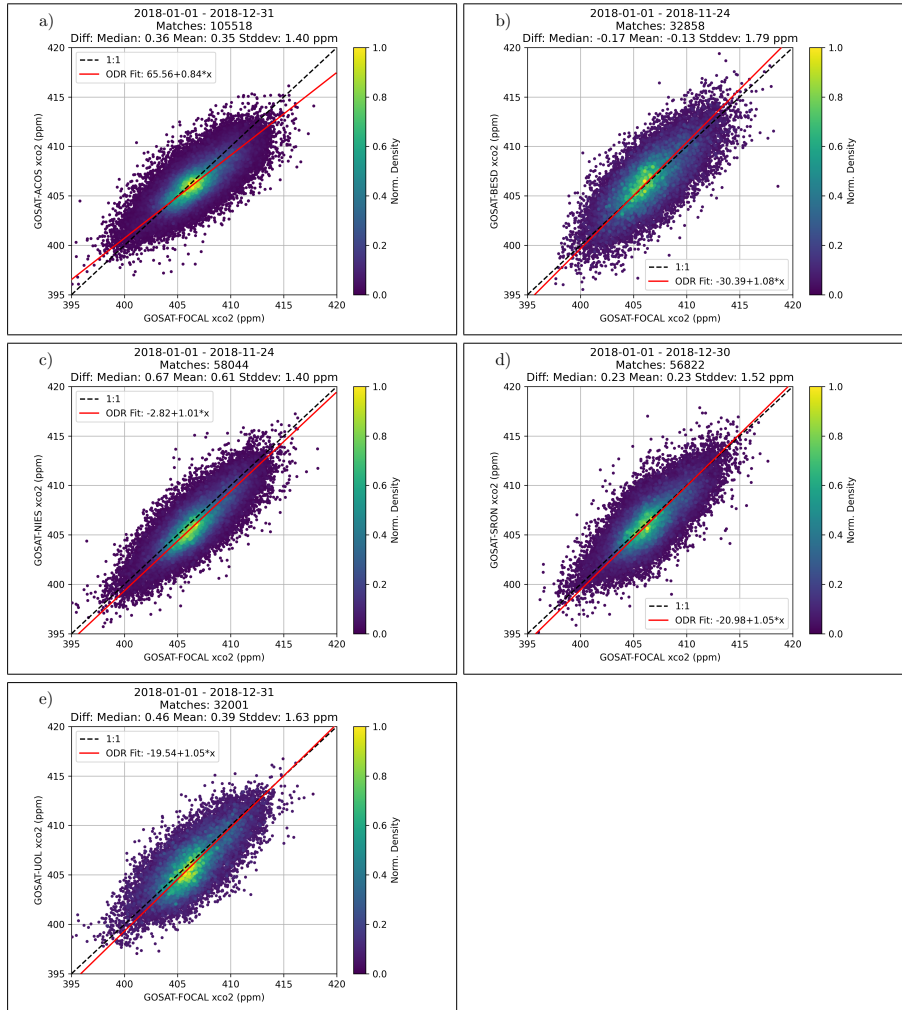
Figure 14. Comparison of GOSAT-FOCAL data (x axis) from 2018 with other GOSAT data (y axis). The colour of the data points corresponds to the density of data points at that location (normalised to a maximum value of 1). The dashed line corresponds to perfect agreement. The red line shows the result of a linear fit using the Orthogonal Distance Regression (ODR) method. The total number of collocated data as well as median, mean and standard deviation of the XCO_2 differences between the two data sets are given in the title of the sub-plots. a) FOCAL vs. ACOS b) FOCAL vs. BESD. c) FOCAL vs. NIES. d) FOCAL vs. SRON. e) FOCAL vs. UoL.
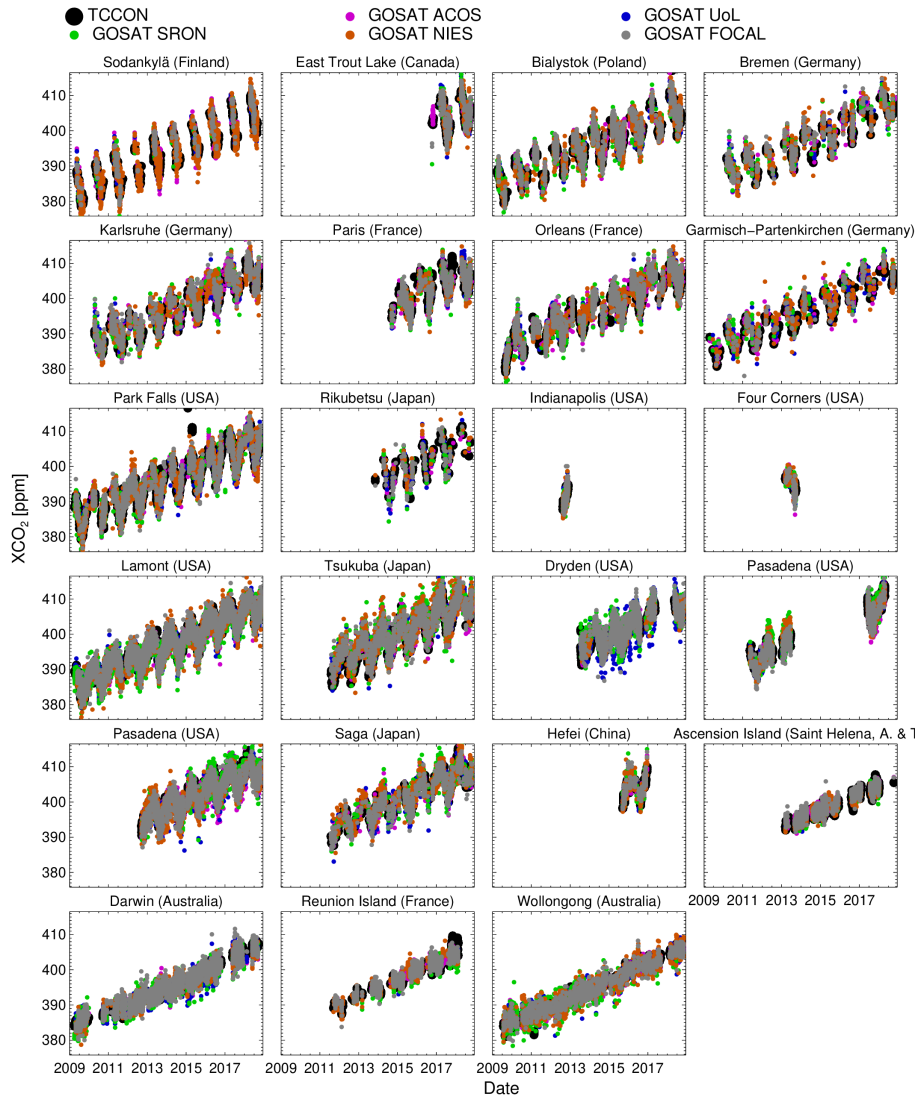
Figure 15. Time series of collocated GOSAT data at various TCCON sites for different data products including the new GOSAT-FOCAL data set.
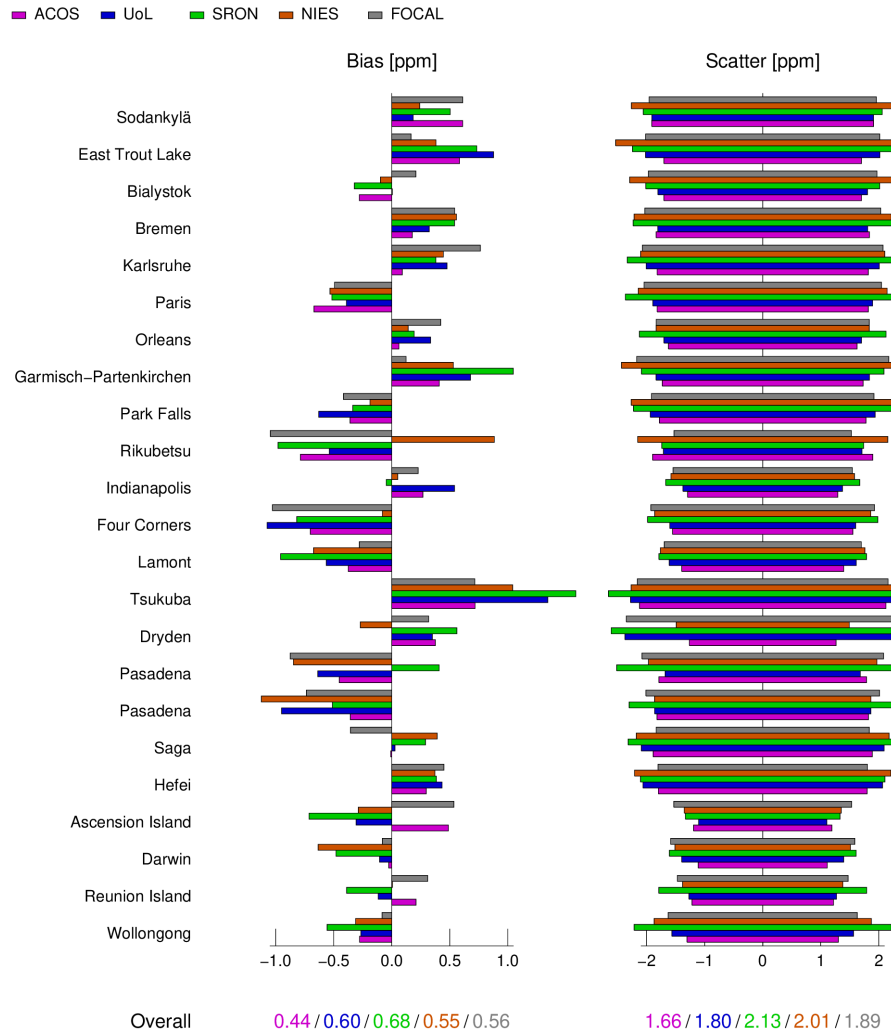
Figure 16. Overview of TCCON validation results for GOSAT.
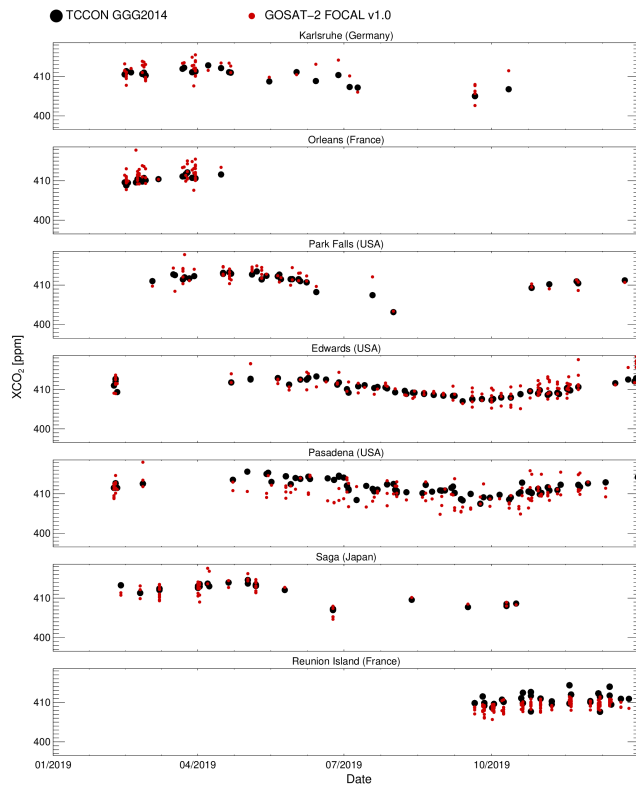
Figure 17. Time series of collocated FOCAL GOSAT-2 data at various TCCON sites.
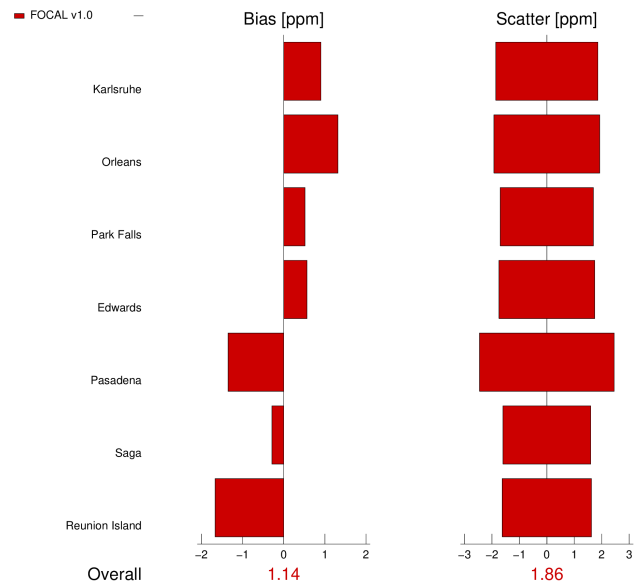
Figure 18. Overview of TCCON validation results for the GOSAT-2 FOCAL product.
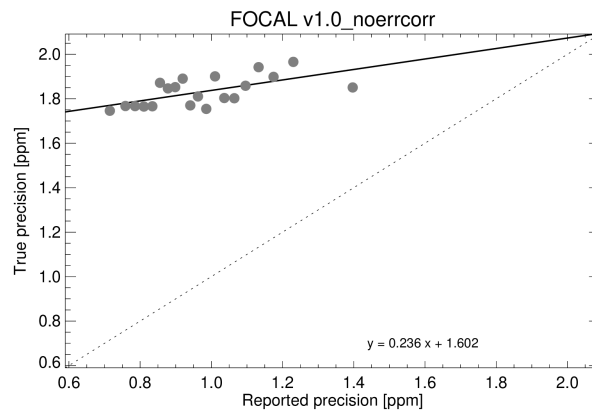
Figure 19. Comparisons of the (binned) original XCO_2 errors (reported precision without correction) of the GOSAT-FOCAL product with estimated errors based on collocated TCCON data (true precision).

Figure 20. Gridded monthly mean time series of different GOSAT XCO_2 products. Left: Time series of mean XCO_2 for four different regions (from top to bottom: Global, northern hemisphere, tropics, southern hemisphere). Right: Corresponding differences to the GOSAT-FOCAL product.

Table 1. TCCON stations used in this study.

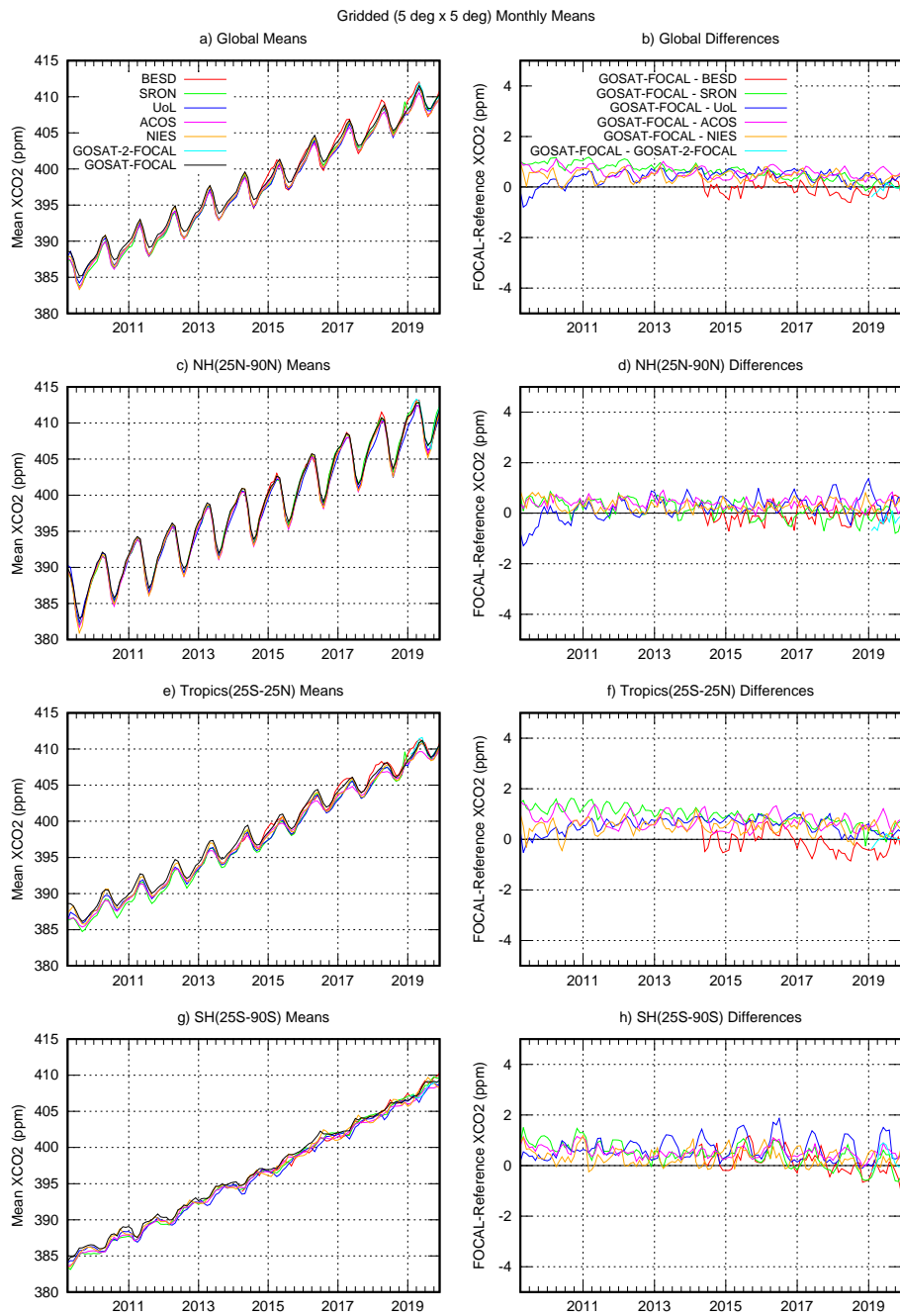| Site	Lon. (deg)	Lat. (deg)	Elev. (km)	Reference(s)
Ascension Island (SH)	-14.33	-7.92	0.01	Feist et al. (2014)
Bialystok (PL)	23.03	53.23	0.18	Deutscher et al. (2019)
Bremen (DE)	8.85	53.10	0.04	Notholt et al. (2019a)
Burgos (PH)	120.65	18.53	0.04	Morino et al. (2018b)
Darwin (AU)	130.89	-12.42	0.03	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)
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. (2014)
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. Pre-processing filter limits.

Filter	Value
GOSAT quality flag	"good" or "poor"
GOSAT-2 quality flag	"good", "fair" or "poor"
Maximum solar zenith angle	70°
Maximum latitude	70°
Minimum SNR	10
Maximum ~~cloud~~ effective albedo	0.7
Maximum water vapour ~~path~~ filter	4.0

Table 3. Parameters for cloud filtering.

Effective Albedo		
GOSAT Band	Waveno. Range (cm^{-1})	Irradiance $(W/cm^2/s/cm^{-1})$
SWIR-1	13190–13210	7.4e-6
SWIR-2	6267–6279	6.0e-6
SWIR-3	4800–4810	4.3e-6
Water Vapour Filter		
GOSAT Band	Waveno. Range (cm^{-1})	
SWIR-3	5176–5193	

Table 4. Definition of GOSAT/GOSAT-2 spectral fit windows (same for S and P). Windows 7 and 8 are only available for GOSAT-2.

No.	Primary target	Waveno. range (cm^{-1})	Considered gases
1	SIF	13170 – 13220	O_2
2	O_2	12930 – 13170	O_2
3	HDO	6337 – 6410	CO_2, H_2O, HDO, CH_4
4	CO_2	6161 – 6297	CO_2, H_2O, HDO, CH_4
5	CH_4	5945 – 6135	CO_2, H_2O, HDO, CH_4
6	CO_2	4801 – 4907	CO_2, 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 5. State vector elements and related retrieval settings. A-priori values are also used as first guess. "Fit windows" lists the spectral windows (see Tab. 4) from which the element is determined. "all" means that an element is determined from all fit windows of the specified polarisation. "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	all S	0.2	1.	Layer height (pressure), S
tau_sca_0_s	all S	0.01	0.1	Optical depth, S
ang_sca_s	all S	4.0	1.	Ångström coefficient, S
pre_sca_p	all P	0.2	1.	Layer height (pressure), P
tau_sca_0_p	all P	0.01	0.1	Optical depth, P
ang_sca_p	all P	4.0	1.	Ångström coefficient, P
		Polynomial coefficients (surface albedo)		
poly0	each	est.	0.01	estimated surface albedo
poly1	each	0.2	0.1	
poly2	each	0.1	0.1	not in SIF window (1)
		Spectral corrections		
wav_shi	each	0.0	0.1	Wavenumber shift
wav_squ	each	0.0	0.001	Wavenumber squeeze

Table 6. Parameters of GOSAT noise model.

Fit window	s	δF	a_0	a_1	a_2	NSR range
S polarisation						
1	1.12	2.17e-03	9.369e-05	1.613e-01	-9.185e-01	0.003–0.049
2	1.07	5.50e-03	1.183e-03	2.557e-02	1.107e+00	0.003–0.047
3	1.14	3.61e-03	5.241e-04	1.251e-01	-6.776e-01	0.003–0.043
4	1.07	3.37e-03	5.480e-04	7.250e-02	3.716e-02	0.003–0.041
5	1.07	3.58e-03	8.836e-04	3.433e-02	8.853e-01	0.003–0.047
6	1.00	7.12e-03	1.680e-03	-9.060e-03	1.190e+00	0.001–0.047
P polarisation						
1	1.13	2.42e-03	5.961e-04	8.736e-02	6.867e-01	0.003–0.049
2	1.05	7.50e-03	3.177e-03	-1.109e-01	2.711e+00	0.003–0.049
3	1.21	3.17e-03	4.909e-04	1.226e-01	5.539e-02	0.003–0.037
4	1.09	3.33e-03	6.725e-04	4.661e-02	1.002e+00	0.003–0.035
5	1.04	3.58e-03	6.457e-04	5.710e-02	2.663e-01	0.003–0.039
6	1.00	6.96e-03	1.488e-03	-9.996e-04	1.262e+00	0.003–0.049

Table 7. Parameters of GOSAT-2 noise model.

Fit window	s	δF	a_0	a_1	a_2	NSR range
			S polarisation			
1	0.90	3.65e-03	5.895e-04	2.314e-01	-1.524e+01	0.003–0.009
2	0.94	5.21e-03	1.143e-03	1.352e-02	4.058e+00	0.003–0.009
3	1.20	3.14e-03	3.972e-04	2.756e-01	7.753e+00	0.001–0.009
4	1.08	5.25e-03	2.491e-04	2.683e-01	-4.440e-01	0.001–0.007
5	1.06	4.04e-03	2.184e-04	4.112e-01	-2.730e+01	0.001–0.007
6	1.01	4.73e-03	6.001e-04	4.469e-01	-2.822e+01	0.001–0.011
7	1.16	7.53e-03	1.289e-03	3.984e-01	-1.377e+01	0.001–0.009
8	1.11	9.34e-03	9.305e-04	5.126e-01	-2.263e+01	0.003–0.017
			P polarisation			
1	0.96	2.83e-03	8.010e-05	2.856e-01	-9.105e+00	0.003–0.017
2	0.97	6.08e-03	2.258e-03	-1.191e-01	6.365e+00	0.003–0.015
3	1.19	3.20e-03	6.571e-04	9.767e-02	1.049e+01	0.001–0.011
4	1.10	5.25e-03	3.868e-04	2.064e-01	-1.886e+00	0.001–0.009
5	1.08	4.17e-03	6.688e-05	4.935e-01	-3.445e+01	0.001–0.009
6	1.02	4.68e-03	1.181e-03	1.123e-01	1.245e+00	0.001–0.015
7	1.01	7.11e-03	1.907e-03	-3.405e-02	1.012e+01	0.003–0.015
8	1.10	9.52e-03	2.093e-03	1.632e-01	-2.418e+00	0.003–0.021

Table 8. Basic filter parameters.

Filter	Range for valid data
Good convergence	$\chi^2 \leq 2$
RSR (each fit window, S&P)	below outlier limit
Scattering layer height (S&P)	0 to 1
Ångström coefficient (S&P)	1 to 5
Scattering layer optical depth (S&P)	0 to 0.02
XCO_2 error	0 to 2.0 ppm

Table 9. Bias filter limits.

Filter	Range for valid data
GOSAT land	-6.9 to -2.9 ppm
GOSAT water	-8.1 to -4.1 ppm
GOSAT-2 land	-4.0 to 0.0 ppm
GOSAT-2 water	-5.5 to -1.5 ppm