The Total Carbon Column Observing Network's GGG2020 Data Version

Response to Referee #1 (Gretchen Keppel-Aleks)

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Thank you to Dr. Keppel-Aleks for her positive review of this manuscript's importance and her careful consideration of how to improve its value as a reference for our data product. We have done our best to address the comments made. Below, comments from the reviewer are in red, our responses are in blue, and quotes of the manuscript are in black. Unless otherwise stated, line, figure, table, and section numbers used in comments and responses refer to the *original* manuscript while such cross-references in quotes of the new version of the paper refer to the *revised* version.

The paper does presuppose knowledge of the network's goals and past versions of the data. For example, line 46 casually states that there is a 0.25% accuracy needed for greenhouse gas data, but this is not motivated in the next nor cited from another source. It could be nice to provide a brief retrospective of the defined needs and past performance for TCCON's precision/accuracy, noting that the precision needs for validation of satellite instruments and for carbon cycle science could be different.

We have added two new paragraphs to the introduction:

> "The need for updates to the retrieval algorithm used by TCCON has been largely driven by the need for increasingly high accuracy and precision of total column greenhouse gas (GHG) data for carbon cycle science and satellite validation. GHG measurements require quite high precision to distinguish signals from anthropogenic, terrestrial, or oceanic processes from the background mixing ratios. The 2018 National Academies decadal strategy recommends random and systematic errors for CO_2 be less than 1 and 0.2 ppm ($\sim 0.25\%$ and $\sim 0.05\%$), respectively and likewise less than 6 and 2.5 ppb ($\sim 0.3\%$ and $\sim 0.1\%$), respectively for CH_4 (National Academies of Sciences, Engineering, and Medicine, 2018, Table B.1, question C-3, p. 601). Future space-based CO_2 observing missions are striving for even greater precision; for example, CO2M has a stated goal of 0.7 ppm precision and < 0.5 ppm systematic error in X_{CO_2} (ESA, 2020). The increasingly stringent precision requirements for carbon cycle science and satellite validation demands that ground based networks, such as TCCON, continue to refine their data to support these requirements.

> A second factor driving improvements in the retrieval is the emergence of portable, low resolution solar-viewing FTIR instruments such as EM27/SUNs. These instruments can be deployed to areas that cannot support a full TCCON site, and are also affordable enough to be deployed in greater density around locations of interest (e.g. cities). This capability complements the higher precision and accuracy data produced by TCCON. To facilitate comparisons between TCCON and EM27/SUN data, it is beneficial to use the same retrieval for both. Improvements to handling of EM27/SUN interferograms (§4.3) have been added."

It might be helpful to provide a table of contents at the end of the introduction, to let the reader know what the main sections of the paper are (e.g., 2 = new Xgas, 3 = Updated spectroscopy). Since many readers will not read the paper end-to-end, this could make the manuscript more effective as a reference.

Done; this is the new Table 1. We have also added a new figure with a flowchart of the components of GGG and the data delivery (new Fig. 1).

While reading the paper, I thought it could be helpful for the authors to tabulate the remaining/known issues with the GGG2020 data that the next version of GGG will attempt to address. For example, the XCO2 vs Xluft dependence or the T-dependence of N2O retrievals. A summary section is included at the end of the paper, however, so this might be unnecessary, but it would be helpful to note that this section is coming in the table of contents so the reader knows it is coming. On the other hand, it could be helpful, to summarize the known issues in a compact format (table, or a call-out box rather than just another section of the paper) if the authors think it could help the user community avoid author-anticipated pitfalls when interpreting the data.

We have added Table 6 in the conclusion.

Somewhat similarly, when I read the error budget section, I noted that a table would be helpful, and there was a table at the end. It is great that the paper is so thorough, but adding a bit of organization to let the reader know that something is coming a bit later on would be very helpful.

We added a sentence at the end of the Sect. 8 introduction that points to this table:

> "Each source of uncertainty included in our error budget is described below. **Table 5 towards the end of this section summarizes the error budget for the primary TCCON products.**"

Line 111: I am curious the extent to which the linelists have been empirically adjusted. For example, how many weak lines have been added based on the empirical identification process described in this paragraph? It would also be interesting if the paper noted how/whether this information gained from the high resolution TCCON spectra flows back to other groups in Earth/sun remote sensing.

It is difficult to summarize the extent of the changes to the linelists, since these changes involve adopting new parts of the HITRAN linelists, adding/removing/shifting lines, etc.

We've instead tried to summarize the improvement in CO_2 at least with statistics of the mean spectral residuals and bias calculated from lab spectra with known CO_2 amounts. This is table 3 in the revised paper. In addition to this table and a paragraph explaining it, we have added a short paragraph on how these improvements in spectroscopy are communicated to the HITRAN group:

> "Improvements to the telluric linelists are communicated to the HITRAN group through spectroscopic evaluations, posted to `https://mark4sun.jpl.nasa.gov/presentation.html` (last access 31 Jan 2024). Such evaluations are also performed on candidate linelists developed by the HITRAN group to provide feedback on the performance of those linelists before they are adopted."

Line 118: refers to Mendonca 2016 and Devi 2007ab, which leads me to believe that these are the lineshapes that are being used in the 6220 and 6339 cm-1 CO2 bands but this is not explicitly stated.

We have added a table to the appendix that lists all the GGG2020 windows and this includes whether gases in that window include non-Voigt data. We point to this at the end of the first paragraph of Sect. 3.2:

> "...quadratic speed-dependent Voigt (qSDV) with line mixing (LM) code from Tran et al. (2013) was implemented into forward model of GGG (Toon, 2022). **Tables A2 and A3 list the frequency windows used in GGG2020, and contain columns identifying which windows include speed-dependent and line mixing lineshape information**"

Line 122: What is the metric the authors used to determine that the new spectroscopy and line shape improved "the quality of XCO2 retrievals in this spectral region" ?

We have clarified that this means spectral RMS, as mentioned earlier in the paragraph:

> "...the spectroscopic parameters from Benner et al. (2016) are used with the qSDV and first order LM to calculate absorption coefficients. This resulted in improving the quality of XCO_2 retrievals **(i.e. reducing the spectral fit RMS)** from this spectral region. New spectroscopic studies aimed at improving CO_2 absorption coefficient calculations..."

Section 3.3: The empirical process to optimize the O2 line widths was very detailed, and I had to read it a few times. I am not sure how the text could be more clear given the multiple interdependent constraints. The figures here were very helpful in communicating the approach. One minor comment is that the allusion to T700 as a metric for synoptic scale meteorology doesn't seem to fit (since a relationship between non-oxygen gases and T700 represents real variability whereas with O2 it is a spurious relationship). It might be more clear to say that T700 was used as a temperature metric because this value is already saved with the observed spectra since it has also been applied for downwind scientific analyses.

T700 isn't saved in the spectra for GGG2020, but was calculated from the a priori profiles for this. We have rewritten this sentence as follows:

> "Our rationale was that the temperature dependence of X_{luft} was the most important error to eliminate, thus minimizing its magnitude took priority. T700 is taken from the a priori meteorology data, **and was chosen on the assumption that this is a reasonable metric for temperature variations in the free troposphere containing the majority (∼ 60%, 800 to 200 hPa) of the O_2 column.**"

Line 178: The sentence about minimizing the variance in Xluft rather than the average value was confusing to me (perhaps because the sentence is pre-empting an argument that didn't occur to me – I'm not sure why it would be useful to minimize the average value).

We've added a sentence to clarify:

> "...rather than the pressure and temperature effects on line width adjusted in this initial experiment. **Therefore, while we ideally want $X_{\text{luft}} = 1$, this first step was not optimizing the spectroscopic parameters that can achieve that. We do adjust the O_2 line strengths separately, as noted at the end of this section.**"

Section 4.3: The reference to trace gas profile updates here was not alluded to in the introduction; perhaps mention ginput in the introductory section

We didn't include any list of updates to the algorithm in the introduction. We believe that now the table of contents serves that purpose; it includes a mention of the meteorology and trace gas profile updates.

Line 251: Clarify whether the DIP metric is reported for users to consider, or is an active filter employed by the TCCON team prior to reporting data. Upon the first reading, it seemed like it was a diagnostic, but I later realized (Line 940) that it is actively used in the filtering process.

We have edited the second-to-last paragraph in this section to make this clear:

> "**We now use the DIP diagnostic during the quality control step to identify data affected similarly by nonlinearity. Once such data is identified,** the correction process **described in the previous paragraph** is applied to **the afflicted data.**"

Line 275 "igram" should be "interferogram", I think.

Fixed.

Line 307: The need to phase correct the interferogram is clear, but it is not clear why computing a spectrum using both the long and short arm of the interferogram is "more efficient" than only using the long arm. Please add a brief sentence to clarify.

This just avoids discarding useful data, but this is only used when processing double-sided interferograms. Since the main use case with double-sided interferograms is EM27 data, we have changed this paragraph to be clearer:

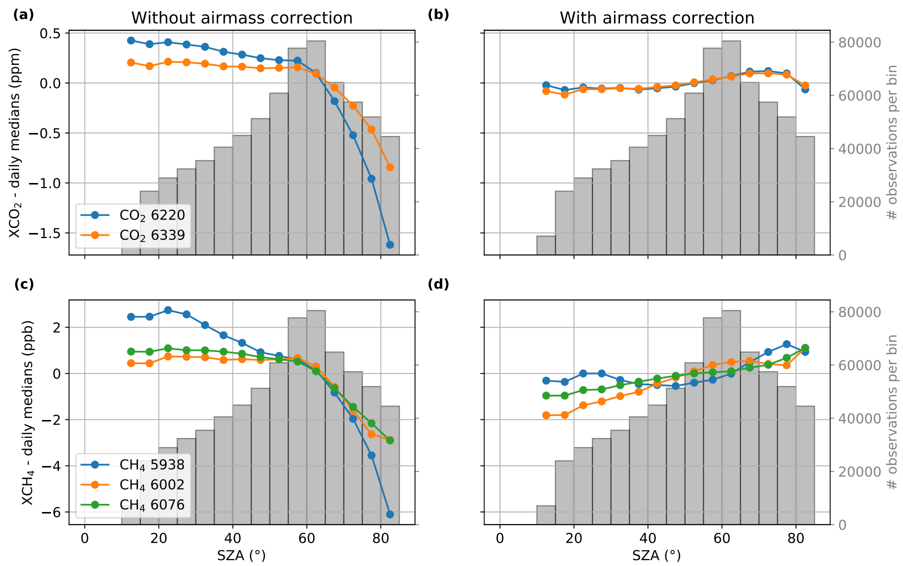

Figure R1: The updated Fig. 5 (now Fig. 10) showing the efficacy of the airmass correction.

> "I2S now has the capability to process interferograms as single sided (using data only from one side of ZPD, usually the long arm) or double sided (using data from both sides of ZPD, the long and short arms). When processing an interferogram as double sided, the optical path difference (OPD) on either side of ZPD must be the same. This means that for standard TCCON processing, I2S will always choose to process the interferogram as single sided, because the long arm is much longer ($\geq$ 45 cm) than the short arm (typically 0.2 to 5.0 cm). However, for spectrometers such as the EM27/SUNs where the OPD is more symmetrical about ZPD, I2S can process the interferogram as double sided, which avoids discarding useful data from the short arm."

For section 7.1 on the airmass correction, the description of the ACDF was a bit confusing. There were quite a few variables introduced, and some might be redundant. For example, my understanding is that alpha and ACDF are the same? And that c3 is closely related to these (just that it has a daily fitted value whereas alpha is the mean of all c3's), so perhaps there is some notation that could be used to show this more clearly (e.g., calling it alpha_i, or alpha_daily)?

We replaced alpha with "ADCF" directly in the equations and renamed the c's to c_{mean}, c_{asym}, and c_{ADCF} to more directly communicate their meaning.

Figure 5: Would it be possible to show panels with the corrected data (side-by-side panels or overlaid if that isn't too messy) to show the result of the procedure?

Done. We have also added background bar plots to indicate the number of data points contributing to each bin, so as to allow readers to understand that some of the low and high SZA behavior is due to having less data available.

Figure 6: It appears that the value selected for g in the 6339 cm-1 window is 45 deg,

which is at the margin of the allowable parameter space. This suggests the optimization hasn't converged, and may reflect that the functional form chosen is not appropriate. Can the authors comment on this?

While it may not have fully converged, we can see from the background color (representing the quantity being minimized) that the final solution is in the middle of a part of the parameter space where the metric to be minimized is already near 0. In fact, because both panels of this figure use the same color map, we can see that the 6339 cm-1 window's standard deviation is overall lower than the 6220 cm-1 window. That suggests instead to us that the 6339 cm-1 window can be well corrected with a variety of values for g and p. That is borne out by the newly added panels for the previous figure (now fig. 6) which show that the CO2 airmass correction is very effective, leaving only a very minor variation in XCO2 with airmass for both windows.

Figure 8 and 9: Please increase the font size on these figures.
Done.

Section 7.2: perhaps clarify whether the sj are the same for all sites and times.
We have added:

> "Thus, while GGG2020 retains the capability to compute the s_j values on-the-fly, the s_j values are prescribed for standard TCCON processing, **and all sites use the same s_j values.**"

Line 450: The vertical scale has been changed from 70 uniform levels to one in which the level separation increase away from the surface. Can the authors comment on how this change impacts the error associated with the stratospheric extrapolation?

We have previously shown (Laughner et al., 2023) that the a priori profiles used for this extrapolation have very good agreement with AirCore profiles in the lower stratosphere. Therefore, any small loss in accuracy due to the larger spacing should be more than offset by the improvement in the quality of the profiles themselves. We have edited this bullet point to say:

> "extend the profiles' tops to 70 km altitude using the standard GGG2020 priors **(shown in Laughner et al. (2023) to have good agreement with in situ profiles in the stratosphere)** and to the surface by extrapolation or use of surface data,""

Line 475: how frequently is a negative Xgas retrieved, and are there any general conditions under which this occurs?

Depending on the gas, this is between 0 and 1% of the spectra in the time windows around the in situ profiles (0.7% for CO2, 0.1% for CH4, 0% for CO and H2O). Because this happens so infrequently, we consider these to be outliers that should be removed. With so few data points to investigate, it is difficult to determine if there is any consistent reason this occurs; however, it probably happens when a cloud interrupts an already-started interferogram.

Figure 11: Could this be bigger and could the yellow color be replaced with a more saturated hue?

Done. We reorganized the panels to allow them to be larger as well.

Figure 12: Does the orange line (X2019+VarO2 – X2019) imply that there is a 0.2 ppm draft in the X2007 retrievals that do not account for variable oxygen, or is this partially corrected for by the slope of the in situ correction since XCO2? Could a residual error be estimated due to neglecting the trend in O2?

Yes, the orange line does imply a drift, and it is not corrected for by the in situ scaling, as that can only correct for the mean error in O2 mole fraction among the retrievals used in the in situ comparisons. That line is the residual error that comes from neglecting the O2. Since we now provide data fields in the public files that include the variation in O2 mole fraction, however, we would recommend users update to these new fields rather than trying to estimate the effect of the O2 mole fraction.

Equation 10: This is another equation where the key parameter is alpha, but with different meaning. Perhaps a different variable could be chosen so that the variables used in the paper have a unique definition.

Since we changed alpha to ADCF in sect. 7.1, this should be unique now.

The error budget was very thorough, but I do not believe Fig. 17 was referenced in the text. This was the figure I found least informative, so perhaps it could be removed completely.

This is referenced in the "Instrument Line Shape" section describing how the sensitivity tests were performed, so we prefer to keep this figure.

References

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