TCCON GGG2020 switch to GEOS IT met products

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Abstract

The GGG2020 TCCON data product relies on the Goddard GEOS product for a priori meteorological information. In particular, it was developed with the GEOS FP-IT (Forward Processing for Instrument Teams) product, as we required the longer record of FP-IT (circa 2000 on) compared to the more recent FP product (circa 2013 on). In 2023, we were informed that the FP-IT product would be succeeded by the GEOS IT product. Due to the effort required to perform a full reprocessing of the TCCON data set (\sim 30 sites with records up to 10 years long), it is not practical at this time to redo the GGG2020 retrievals with the GEOS IT input data. Therefore, we have made arrangements to switch our retrievals over to the GEOS IT product starting at midnight UTC, 1 Apr 2024. This date was chosen to coincide with the switch of OCO-2 and -3 processing to also use GEOS IT, rather than GEOS FP-IT. This document describes the testing done to quantify the impact this change will have on the GGG2020 data product.

1 Testing methodology

GGG2020 requires a priori meteorological and trace gas VMR profiles as input to the retrieval. The meteorological data is taken directly from GEOS FP-IT or IT, interpolated to the TCCON site location, and the VMR profiles are either likewise interpolated (H₂O, O₃, CO) or derived from those meteorological values (CO₂, CH₄, N₂O, HF) [1]. To test the impact of the GEOS FP-IT to GEOS IT change, the input files containing these meteorological and VMR data were generated using both meteorology products for four months: Oct 2022, Feb 2023, Apr 2023, and July 2023. These months were chosen to match the months used in OCO-2 testing, so that comparisons between the impact on OCO-2 and TCCON retrievals could be compared if necessary. They also provide one month per season to test if the impact of the change in meteorology varies throughout the year. Specific TCCON sites were directly asked to run retrievals for these months using both meteorology product. These sites were chosen to provide examples in different parts of the world. All TCCON sites were invited to participate if they had the time to. As of April 25, 2024, the participating sites are:

- Pasadena, CA, USA,
- Armstrong, CA, USA,
- East Trout Lake, Saskatchewan, Canada,
- Lauder, New Zealand,
- Lamont, OK, USA,
- Park Falls, WI, USA,
- Paris, France, and
- Sodankylä, Finland.

When calculating differences, observations from the two datasets (i.e. the retrievals done using GEOS FP-IT and GEOS IT) were matched based on their observation time. All differences reported (e.g. Δ Xgas) are GEOS IT minus GEOS FP-IT.

2 Changes to retrieved Xgas values

On average, the change to most of the Xgas products is near zero (XCO being the exception), relative to the typical magnitude of the Xgas values (Table 1, Figs. 1 & 2). While the histograms in Figs. 1 and 2 do show that individual values have significantly more value, the averages over the four months studied mostly regress toward zero. This is the expected behavior; while the change in meteorology will certainly have some random variation at

Site	$\substack{\text{XCO}_2\\\text{ppm}}$	$\substack{\text{XwCO}_2\\\text{ppm}}$	$\substack{\text{XlCO}_2\\\text{ppm}}$	$_{\rm ppm}^{\rm XCH_4}$	XCO ppb	$_{\rm 2D}^{\rm XN_2O}$	$_{\rm ppm}^{\rm XH_2O}$	XHDO ppm
Pasadena	-0.015	0.016	0.042	-0.000089	-8.3	-0.027	1.30	2.10
Armstrong	-0.014	0.0080	0.055	0.000051	-1.98	-0.073	-0.96	-1.8
ETL	-0.022	0.015	0.018	0.00010	-1.5	0.092	0.36	-2.2
Lauder	-0.013	0.0095	-0.016	0.00016	-0.62	0.11	-1.16	-2.0
Lamont	-0.010	0.016	0.053	0.00042	-1.20	0.039	-3.6	-8.1
Park Falls	-0.046	-0.062	0.044	-0.00011	-1.6	-0.040	-0.70	-2.8
Paris	-0.028	-0.022	0.044	0.000078	-6.7	-0.053	-3.0	-1.4
Sodankylä	-0.018	0.016	0.069	-0.00010	-1.1	-0.012	1.5	1.9
Mean	-0.021	-0.0034	0.039	0.000064	-2.9	0.0047	-0.78	-1.8

Table 1: The mean differences in the six primary TCCON Xgas products for each of the sites participating in the test. Units for each gas are given in the header. Note that not all sites have data for each month of the test, therefore some of the variation between sites is due to temporal sampling. The "Mean" row is the mean of the individual sites' means.

each time that will impact the retrieval, we did not expect a systematic change in the meteorological variables or the a priori VMR profiles derived from them that would result in a systematic bias between the two tests. Additionally, the timeseries shown in Fig. 3 and 4 show that, again excepting XCO, the differences are generally consistent month to month. The changes in XH_2O are somewhat more variable in July, but this is likely due to more water in the atmospheric column during the northern hemisphere's summer.

XCO is the exception; it clearly decreases at the Pasadena, Paris, and (to a lesser extent) East Trout Lake and Armstrong sites. The larger changes in XCO are due to the larger impact of the change in meteorology on the CO a priori profiles. CO is one of the gases for which the a priori VMR profile is interpolated directly from the GEOS product. As shown in Fig. 5, the Pasadena site has a very large decrease in the CO priors towards the surface. Similar but smaller decreases can be seen in the Paris and Armstrong profiles, particularly in July. East Trout Lake also has a decrease in the July CO profiles, but of order 50 ppb, so it is difficult to see on the scale of Fig. 5. We expect this is due to changes in the GEOS CO emissions, as Pasadena and Paris are both urban sites, where decreases in the GEOS CO emissions would clearly have strong impacts on the CO profiles. Armstrong, though not an urban site, is close enough to Los Angeles that its CO priors experience influence from Los Angeles emissions at the GEOS grid size. East Trout Lake by contrast is a very rural site. However, the data where it shows a decrease in XCO occur in July 2023, when there were major wildfires across much of Canada. Our hypothesis is that the change to GEOS CO emissions also altered the fire CO emissions, leading to the ~ 50 ppb decrease in lower atmosphere CO in the East Trout Lake July priors.

3 Changes in remaining a priori profiles

Figures 6 to 10 show the changes in a priori pressure, temperature, CO_2 , CH_4 , and N_2O . Pressure and temperature tend to decrease and increase, respectively, near the surface, but

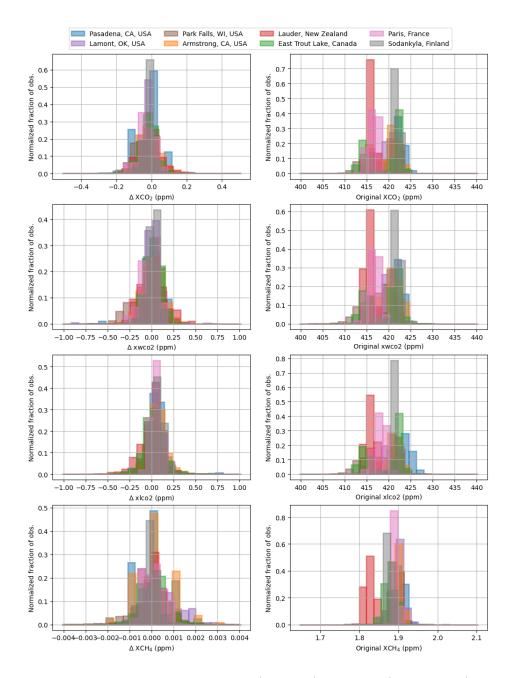


Figure 1: Histograms of the changes in XCO_2 (top row), $XwCO_2$ (second row), $XlCO_2$ (third row), and XCH_4 (bottom row) and their original values. The changes are shown in the left column, the original values in the right. The histograms are normalized such that the sum of all bins equals 1.

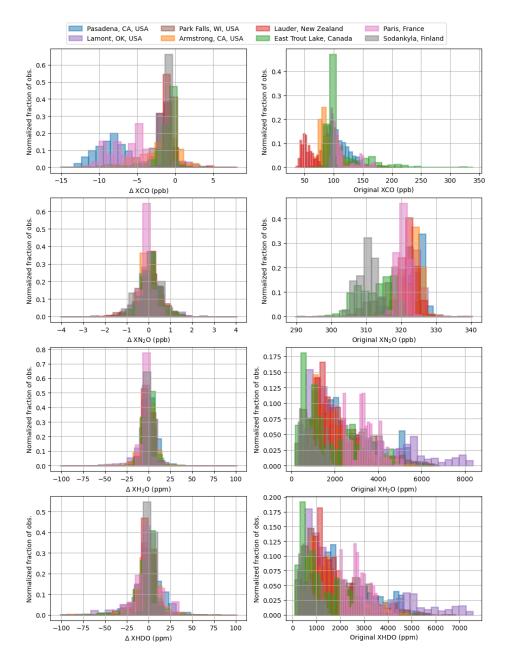


Figure 2: As Fig. 1, but for XCO, XN₂O, XH₂O, XHDO.

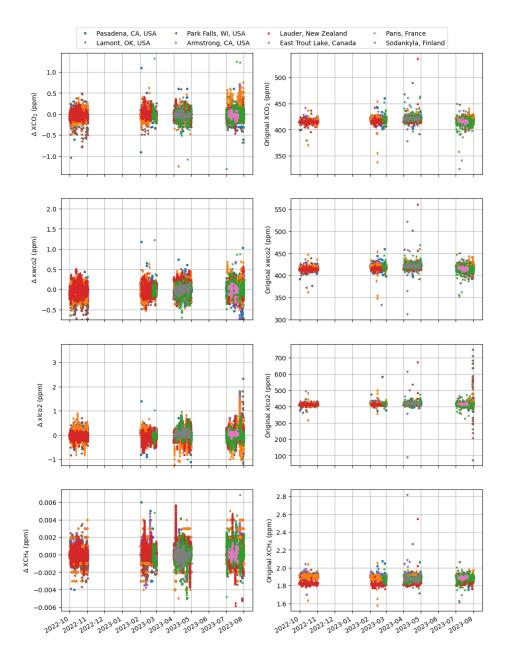


Figure 3: Timeseries of the changes in XCO_2 (top row), $XwCO_2$ (second row), $XlCO_2$ (third row), and XCH_4 (bottom row) and their original values. The changes are shown in the left column, the original values in the right.

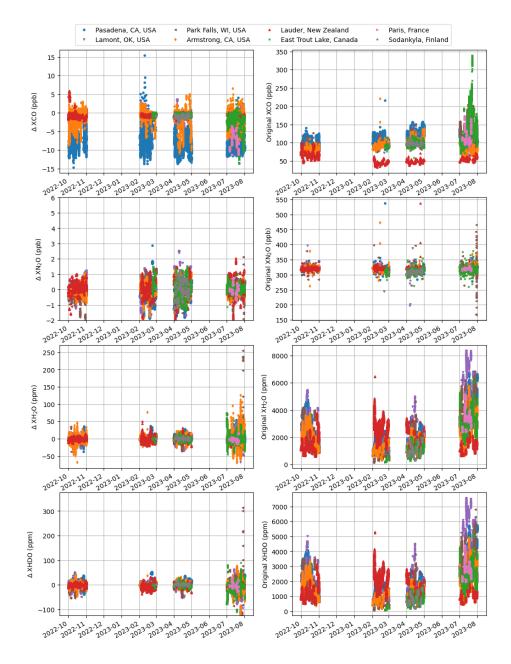


Figure 4: As Fig. 3, but for XCO, XN₂O, XH₂O, and XHDO.

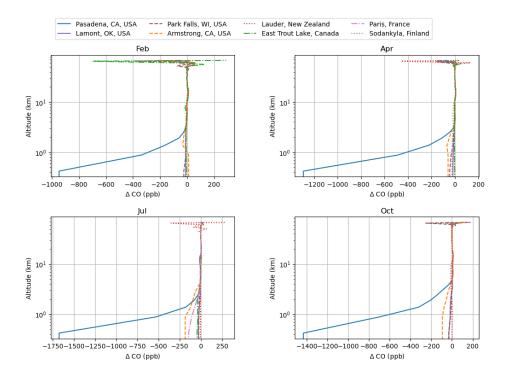


Figure 5: Mean change in the CO a priori profiles for each of the four months in this study. Note that not all sites have data for all months.

by relatively small amounts. Changes in the stratosphere are more variable. The CO_2 , CH_4 , and N_2O profiles, which derive from the pressure and temperature profiles (along with potential vorticity) [1] likewise show minor mean changes near the surface, with more variability in the stratosphere. Given that the troposphere mean changes are small, and the stratospheric changes tend to oscillate around zero, it makes sense that the changes to these prior quantities have little mean effect on the retrieved Xgas values.

4 Conclusions

The change from GEOS FP-IT to GEOS IT as the source of a priori meteorological information for the TCCON GGG2020 data product will produce some random differences in individual observations, but little to no systematic difference for XCO_2 , $XwCO_2$, $XlCO_2$, XCH_4 , XN_2O , XH_2O , and XHDO. Therefore, satellite validation and carbon cycle studies using these products need not be concerned about a step change in the data, so long as a reasonable averaging window is used. Studies using the GGG2020 XCO product should be aware that, especially in urban sites and fire plumes, there likely is a systematic difference. XCO trends that cross the 1 Apr 2024 transition date should note that urban sites, such as Pasadena and Paris, may see a 5 to 10 ppb decrease after that date due to the a priori data.

The TCCON algorithm team is aware of the desirability of reprocessing at least urban sites

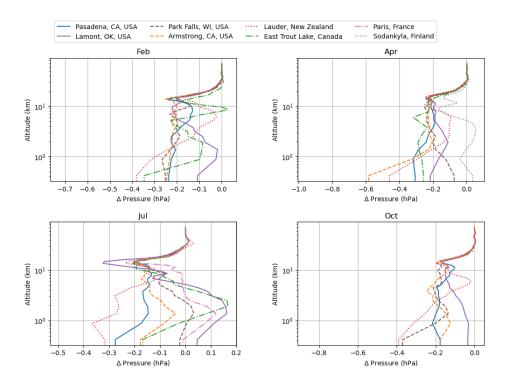


Figure 6: Mean change in the pressure a priori profiles for each of the four months in this study. Note that not all sites have data for all months.

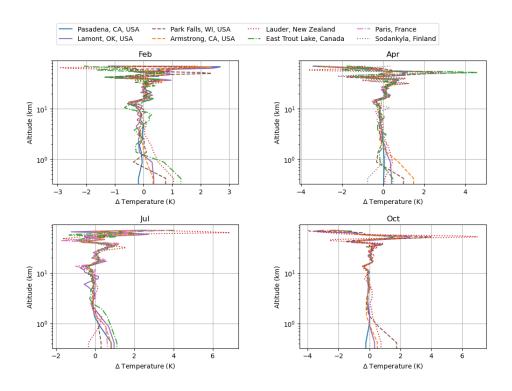


Figure 7: As Fig. 6, but for temperature.

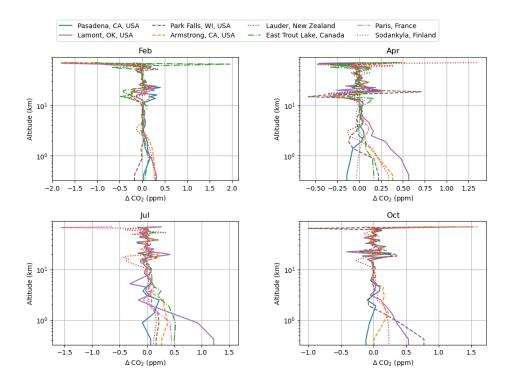


Figure 8: As Fig. 6, but for CO_2 .

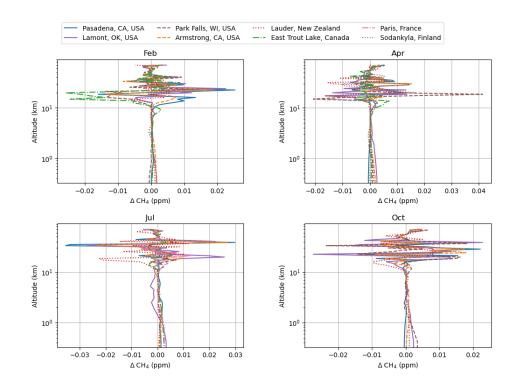


Figure 9: As Fig. 6, but for CH_4 .

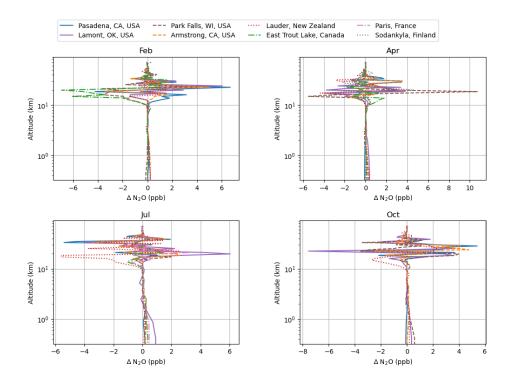


Figure 10: As Fig. 6, but for N_2O .

with GEOS IT a priori information to remove this step change in XCO and reduce the high bias in XCO coming from the urban CO a priori profiles. One current limitation is that doing so would require downloading the full GEOS IT record, which is a prohibitively large amount of data storage for our system. We will explore other options that would overcome this limitation, such as remote access of the GEOS IT product through OpenDAP or migrating to a larger system, in the future. Another limitation is that reprocessing only some sites with different CO a priori profiles would introduce inconsistency in the GGG2020 product until all sites could accomplish said reprocessing. Thus, a full reconciliation of the change in CO a priori profiles may be delayed until the next full TCCON reprocessing with a major update to the GGG retrieval.

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References

[1] Joshua L. Laughner et al. "A new algorithm to generate a priori trace gas profiles for the GGG2020 retrieval algorithm". In: *Atmos. Meas. Tech.* 16.5 (Mar. 2023), pp. 1121– 1146. ISSN: 1867-8548. DOI: 10.5194/amt-16-1121-2023. URL: http://dx.doi.org/ 10.5194/amt-16-1121-2023.