FRM4GHG
Fiducial Reference Measurements for Greenhouse Gases

Deliverable D23 for CCN2
Assessment of HCHO column data from low-resolution instruments (Vertex70 and 125HR low-resolution measurements)

Deliverable:	**D23**
Date:	**30/06/2020**
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Subject:	**ESA-IPL-POE-LG-cl-LE-2015-1129**
Category:	**ESA Express Procurement (EXPRO)**
Our ref.:	**Proposal No. 1129/2015 – Proposal from February 16, 2016, comments from May 27, 2016**

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1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V0.0	2020-06-18	-	Initial version

2 ACCESS LIST

This document is a deliverable "D23: Assessment of HCHO column data from low-resolution instruments (Vertex and 125HR low-resolution measurements)." created for the project FRM4GHG CCN2 and will be submitted to ESA. The document can be downloaded from the project webpage: http://frm4ghg.aeronomie.be.

3 PURPOSE

This document provides the assessment of formaldehyde (HCHO) column data from Bruker Vertex70 and low-resolution measurements performed with the Bruker IFS 125HR in comparison to the HCHO column data from the high-resolution measurements performed with the Bruker IFS 125HR during the FRM4GHG campaign at Sodankylä site for the year 2019.

4 DOCUMENT STRUCTURE

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5 RESULTS

A high-resolution Bruker IFS 125HR Fourier transform infrared (FTIR) spectrometer at the Sodankylä site has been performing regular solar absorption measurements under clear-sky conditions with the liquid nitrogen (LN_2) cooled Indium Antimonide (InSb) detector since 2012. The measurements were performed using a calcium fluoride (CaF_2) beamsplitter and covering a spectral range of 2400 – 3310 cm^{-1}, using a NDSC (Network for the Detection of Stratospheric Change) filter number 3. The total column concentrations of formaldehyde (HCHO) has been retrieved from these measured spectra using a harmonized retrieval strategy which was applied across several other FTIR stations performing similar measurements as discussed in Vigouroux et al. 2018. This paper also includes a detailed discussion on the instrumental setup and retrieval strategy used for the HCHO retrieval for the different FTIR instruments with varying resolutions. The lowest resolution instrument so far was a Bruker Vertex80 which performed measurements with a spectral resolution of 0.075 cm^{-1}.

During the FRM4GHG project we have performed solar absorption measurements under clear-sky conditions at the Sodankylä site with a LN_2 cooled InSb detector with our test instrument, a Bruker Vertex70, at a spectral resolution of 0.2 cm^{-1}. These measurements were compared to the standard high-resolution (0.005 cm^{-1}) measurements performed with a Bruker IFS 125HR from the same location. In addition, we performed low-resolution measurements at 0.2 cm^{-1} with the Bruker IFS 125HR over a one-month period in March 2019. These measurements were performed at the same resolution of the Vertex70 to understand the resolution dependence on the HCHO retrieval results while keeping the same instrumental setup. The retrieval strategy and the results are discussed here.

Selection of micro-windows:
The HCHO signal has a very weak absorption signatures (below 1%) in the infrared spectral region. In the paper of Vigouroux et al. 2018, four micro-windows (mws) as shown below have been used.
Micro-windows – mw1: 2763.42 – 2764.17 cm-1; mw2: 2765.65 – 2766.01 cm-1;
mw3: 2778.15 – 2779.10 cm-1; mw4: 2780.65 – 2782.00 cm-1;
These mws were selected either by avoiding mws with strong interfering lines or by including them only when the fit results to the forward model was very good. In this work the high-resolution measurements with the Bruker IFS 125HR were processed using the same 4 mws strategy.

The low-resolution datasets from the FRM4GHG campaign were first processed using mw3 and mw4 (2 mws strategy). Although these two mws have more interfering species, the HCHO signal is much stronger as compared to the mw1 and mw2. Adding the mws1 and 2 almost do not provide additional information / degrees of freedoms (DOFs) for the high-resolution retrievals. The mw1 and mw2 are very small and therefore for the low-resolution instrument these two mws were removed during the initial test.

An example of solar absorption spectra recorded by the Vertex70, 125HR low-resolution (also labelled as HR125LR) and 125HR for mw3 and mw4 are shown in Figure 1 and Figure **2**, respectively.

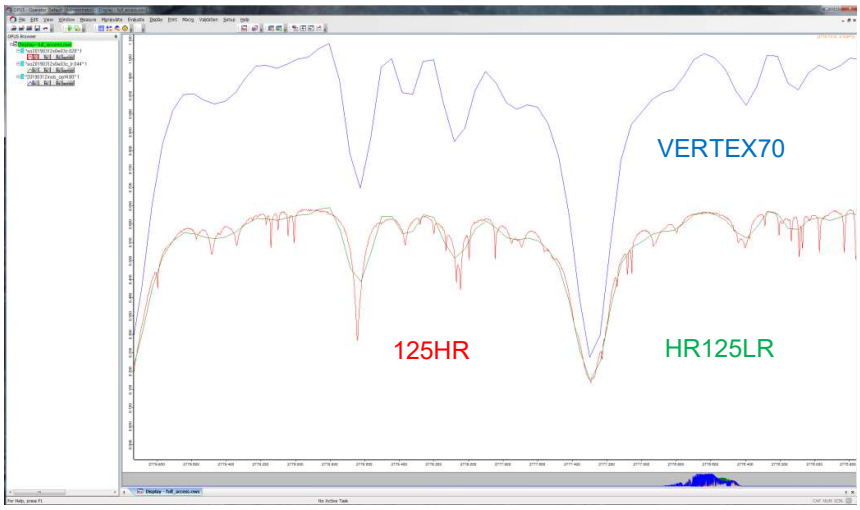

Figure 1: Spectrum from the Vertex70 (blue), HR125LR (green) and 125HR (red) for the micro-window range 2778.15 – 2779.10 cm^{-1}.

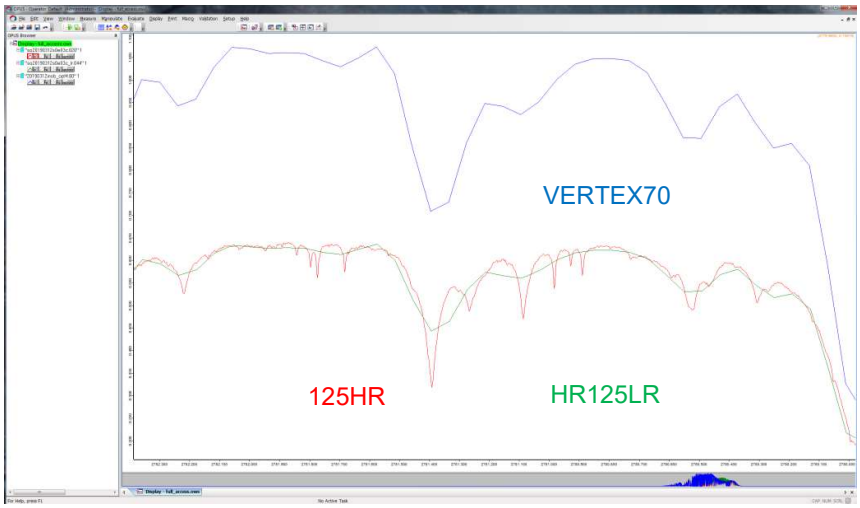

Figure 2: Spectra from the Vertex70 (blue), HR125LR (green) and 125HR (red) for the micro-window range 2780.65 – 2782.0 cm^{-1}.

The time series of the HCHO retrieval results using the 2 mws strategy (mw3 + mw4) from the low-resolution measurements performed with the Vertex70 and Bruker IFS 125HR being compared to the high-resolution measurements with the Bruker IFS 125HR retrieved with the standard 4mws strategy are shown in the top panel plot of Figure 3.The difference is shown in the bottom panel plot.

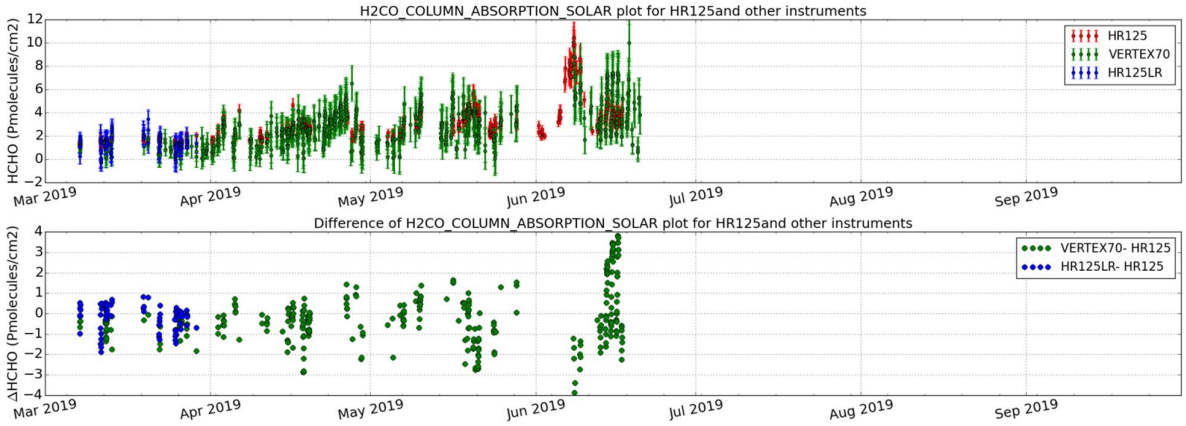

Figure 3: Timeseries of HCHO retrieved with the 2 mws strategy for the low-resolution measurements performed with the Vertex70 (green) and HR125LR (blue) and HCHO retrieved with the 4 mws strategy for the high-resolution reference measurements performed with the HR125 (red).

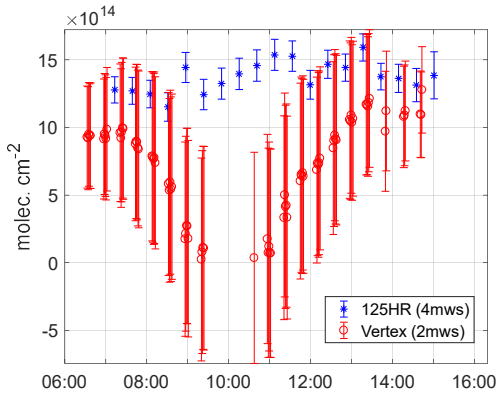

Figure 4: HCHO total column plotted for 12 March 2019 for the 125HR (4 mws strategy) and the Vertex70 (2mws strategy).

The Vertex70 HCHO results with 2 mws strategy shows diurnal artifact (Figure 4) which is not seen in the results of the high-resolution 125HR 4 mws strategy. In order to verify the effect of the retrieval mws, the 4 mws strategy retrieval was done for the Vertex70 measurements. As shown in the left panel plot of Figure 4, the 4 mws retrieval for the Vertex70 improves the diurnal artifact. However, there still remains a large bias with the 125HR which needs to be improved. The right panel plot of Figure 4 shows that the bias is reduced in the 125HR low-resolution retrieved results and follows the same diurnal cycle as the high resulution results. This indicates that the bias seen in the 125HR and the Vertex70 4 mws strategy results does not seem to be due to the lower resolution. The scatter of the 125HR low-resolution measurements is high as compared to the high-resolution measurements.

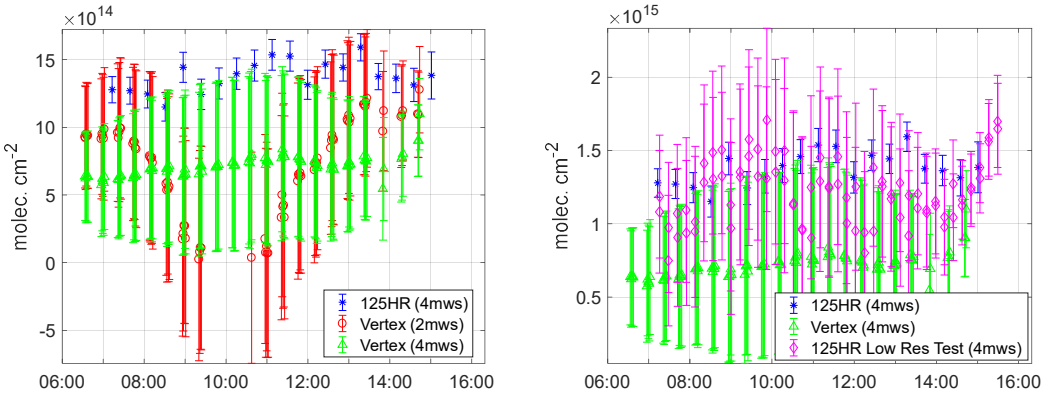

Figure 5: Left - HCHO retrieved from the Vertex70 measurements with 2 mws (red) and 4 mws (green) strategy and compared to the HCHO retrieved with 4 mws strategy from the 125HR measurements (blue) for the same day as in Figure 4. Right – HCHO retrieved with the 4 mws strategy from the low-resolution measurements performed with the 125HR (magenta) and the Vertex70 (green) and compared to the HCHO retrieved with the 4 mws strategy from the 125HR measurements plotted for the same day as in Figure 4.

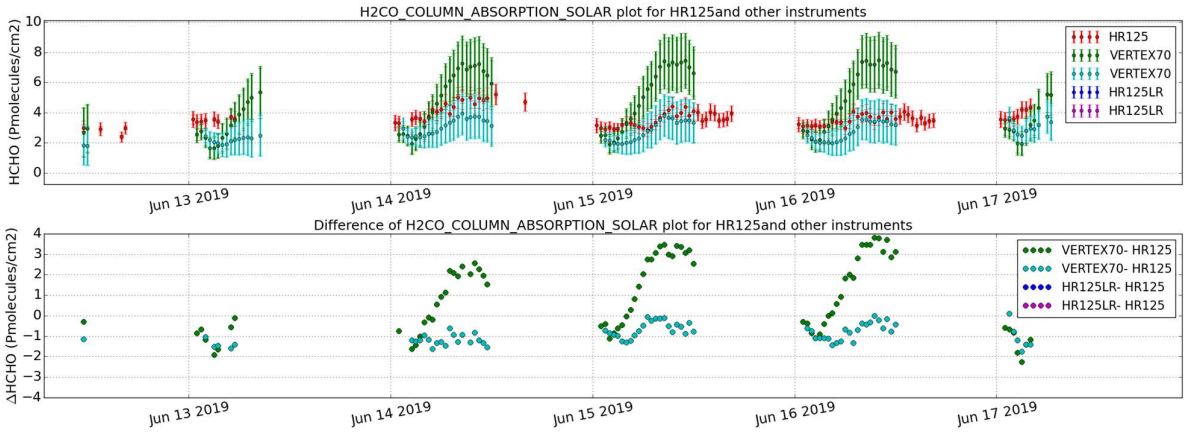

Figure 6: Five day plot in June 2019 (top panel) and bias (bottom panel) of the HCHO retrieved with the 2 mws strategy for the Vertex70 measurements (green) and with the 4 mws strategy from the Vertex70 measurements (cyan) as compared to the high-resolution measurements (red).

The HCHO retrieved with the 4 mws strategy from the Vertex70 measurements shows reduced artifact as compared to the results from the high-resolution measurements with the Bruker IFS 125HR (Figure 6).

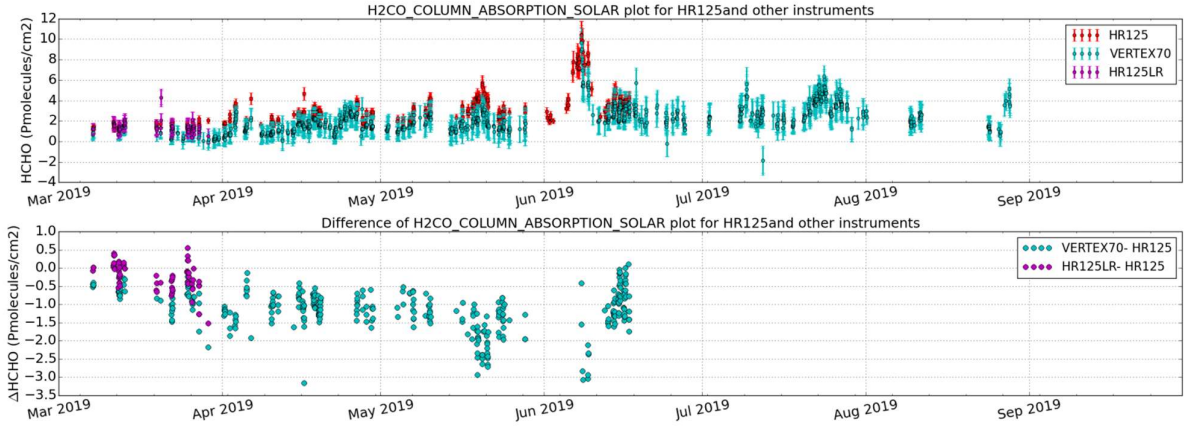

Figure 7: Timeseries (top panel) and bias (bottom panel) of HCHO retrieved with the 4 mws strategy for the low-resolution measurements performed with the Vertex70 (cyan) and HR125LR (magenta) and the high-resolution reference measurements (red).

The plot in Figure 7 shows the improved results with 4 mws case for the low-resolution measurements with both the Vertex70 and the HR125LR datasets. Although the HCHO concentration at the Sodankylä site is low, the HCHO retrieved from the Vertex70 are able to capture the seasonal variability as seen by the high-resolution measurements with the Bruker IFS 125HR. However, there is some residual bias and high scatter in the low-resolution data which needs to be further improved. The large bias does not seem to be due to the lower resolution: the 125HR instrument used in the low-resolution configuration does not show this high bias.

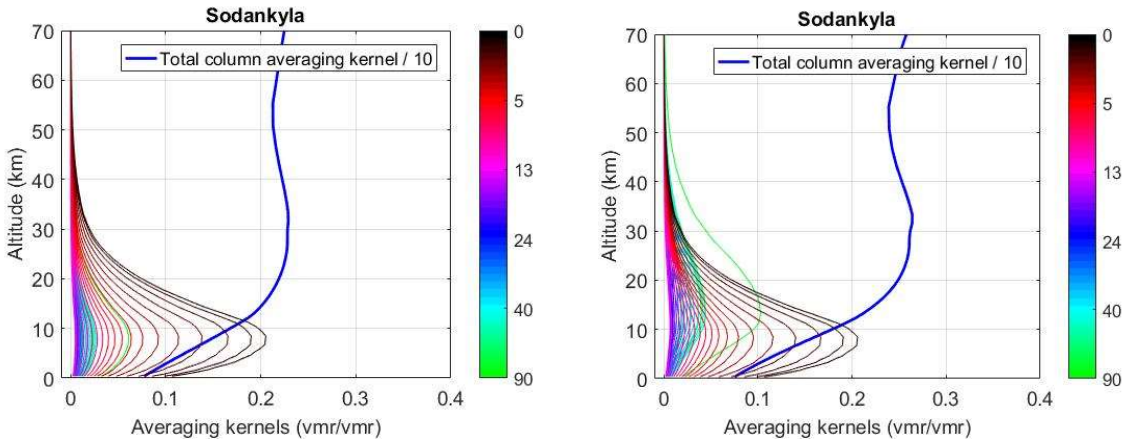

Figure 8: Left - Averaging kernels for the Vertex70. Right - Averaging kernels for the Bruker IFS 125HR. The total column averaging kernel is shown as a thick blue line (divided by 10 for clear visibility). The color code for the different averaging kernels depending on their altitude is given in the color bar with the unit of kilometers.

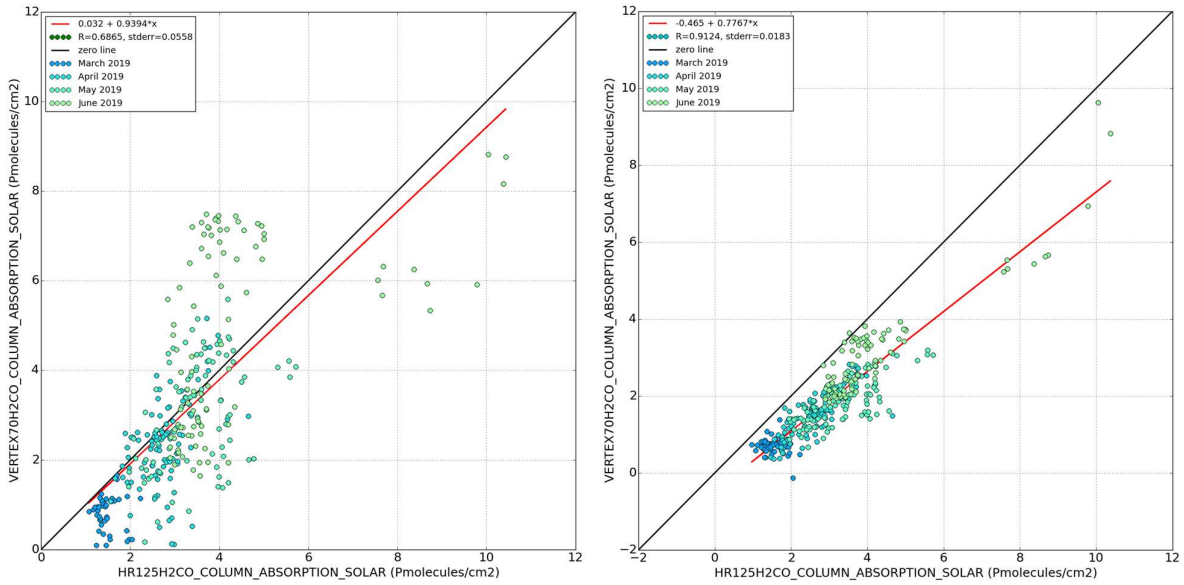

Figure 9: Left – Correlation plot between HCHO retrieved with the 4 mws strategy for the high-resolution measurements vs the 2 mws strategy with the Vertex70 measurements. Right – the same plot as on the left but the HCHO was retrieved with the 4 mws strategy for the Vertex70 measurements.

The HCHO retrieved from the Vertex70 measurements with the 2 mws strategy has a mean bias of -0.163 x 10^{15} molec. cm^2 with a standard deviation of 1.392 x 10^{15} molec. cm^2 and a correlation coefficient of 0.69 with respect to the high-resolution measurements from the Bruker IFS 125HR for the period between March and June 2019. The comparison results with the 4 mws strategy showed an improved correlation value of 0.91 and a reduced scatter of 0.555 x 10^{15} molec. cm^2 with a mean bias of -1.140 x 10^{15} molec. cm^2 for the same time period. The correlation plots for the 2 mws and 4 mws strategy for the Vertex70 with respect to the high-resolution measurements from the Bruker IFS 125HR are shown in the left and right panel plots of Figure 9.

6 SUMMARY AND OUTLOOK

The total column concentrations of formaldehyde (HCHO) have been retrieved from a Vertex70 instrument measuring at low-resolution (0.2 cm^{-1}). The retrievals were performed using two strategies: (1) 2mws (mw3 + mw4) strategy and (2) 4 mws strategy (mw1+mw2+mw3+mw4). The 4 mws strategy improves the diurnal artefact relative to the 2 mws strategy. The 4 mws strategy gives better comparable results with a high correlation coefficient and reduced scatter for the low-resolution data sets measured with the Vertex70 and the Bruker IFS 125HR relative to the high-resolution reference data set measured with the Bruker IFS 125HR. The results from the Vertex70 look promising with some further optimization and improvements needed which are suggested below.

In the future work further optimization of the micro-windows and retrieval strategy for the low resolution has to be done to reduce the scatter in comparison to the high-resolution measurements. We need to investigate the cause of the bias and check if this remains constant such that it can be calibrated by applying a constant calibration factor in comparison to the reference high-resolution measurements. We need to check the dependence of the HCHO retrievals from the low-resolution measurements on the total column of H_2O in the measurements and their dependence on the airmass. We need to investigate if the difference between the HCHO retrieved from the low-resolution measurements using the Bruker IFS 125HR and the Vertex70 might be due to any alignment issue of the later instrument.

7 REFERENCES

Vigouroux, C., Bauer Aquino, C. A., Bauwens, M., Becker, C., Blumenstock, T., De Mazière, M., García, O., Grutter, M., Guarin, C., Hannigan, J., Hase, F., Jones, N., Kivi, R., Koshelev, D., Langerock, B., Lutsch, E., Makarova, M., Metzger, J.-M., Müller, J.-F., Notholt, J., Ortega, I., Palm, M., Paton-Walsh, C., Poberovskii, A., Rettinger, M., Robinson, J., Smale, D., Stavrakou, T., Stremme, W., Strong, K., Sussmann, R., Té, Y., and Toon, G.: NDACC harmonized formaldehyde time series from 21 FTIR stations covering a wide range of column abundances, Atmos. Meas. Tech., 11, 5049–5073, https://doi.org/10.5194/amt-11-5049-2018, 2018.