Carbon monoxide mid- and near infra-red data assessment

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Executive summary

In this task the mid- and near infrared data assessment for carbon monoxide from the two leading FTIR measurement networks NDACC and TCCON are compared. For the three stations Bremen, Izana and St. Denis, which are part of both networks, similar systematic differences in retrieved total columns where found. For the Jungfraujoch station, part of the NDACC network, a new developed retrieval strategy for the near infrared shows less variability compared to NDACC.

Applicable and reference documents

Rodgers, C. D., Inverse methods for atmospheric sounding, Series on Oceanic and planetary physics – vol. 2, World Scientific, 2000.
Toon, G. C., Farmer, C. B., Schaper, P. W., Lowes, L. L., and Norton, R. H.: Composition measurements of the 1989 arctic winter stratosphere by airborne infrared solar absorption spectroscopy, J. Geophys. Res., 97, 7939–7961, doi:10.1029/91JD03114, 1992.

Acronyms and abbreviations

NDACC, Network for the Detection of Atmospheric Composition Change
TCCON, Total Carbon Column Observing Network
FTIR, Fourier Transform Infrared Spectrometer
MIR, Mid-Infrared
NIR, Near-Infrared

1. Introduction

The aim of this report is to investigate the quality and consistency of the two different data products for CO from ground-based FTIR spectrometry. The global measurement networks NDACC and TCCON follow different strategies for the observation and retrieval of CO: they use different retrieval algorithms and different spectral ranges. In NORS, CO data from NDACC will be delivered to the Validation Server, but in the future also the delivery of TCCON-derived CO data could be envisaged. The required pieces of data characterization have already been identified in previous activities within the NORS and the NDACC remote sensing communities.

2. Overview

The contributing sites for this investigation are La Reunion, Jungfraujoch, Izana and Bremen. CO is a target gas for both the NDACC and the TCCON networks.
FTIR NDACC outputs are target profiles retrieved from mid infrared spectra using the SFIT algorithm or the PROFFIT algorithm, which both are implementations of the optimal estimation inversion method or Tikhonov regularization [Rodgers, 2000]. The inversion method allows determining a low resolution vertical concentration profile of an absorber molecule out of a measured spectrum. The total column is the integration of the profile over all altitudes. For the present study, the standard NDACC retrieval settings have been applied; the retrieval microwindows are shown in Table 1.

Table 1. NDACC retrieval windows for CO.

Window [wavenumbers]	Width [wavenumbers]	Interfering gases
2057.70 - 2058.00	0.30	O_3, CO_2, OCS
2069.56 - 2069.76	0.20	O_3, CO_2, OCS
2157.50 – 2159.15	1.65	O_3, CO_2, OCS, N_2O, H_2O

TCCON outputs are retrieved from spectra in the near infrared spectral region using the GFIT algorithm, which uses profile scaling to obtain the vertical total column of the target gas [Toon et. all, 1992]. The input apriori profile is taken from model calculations and not flexible to local concentration changes at specific altitudes. For comparison the standard TCCON settings have been applied, the windows are shown in Table 2.

Table 2. TCCON retrieval windows for CO.

Window [wavenumbers]	Width [wavenumbers]	Interfering gases
4233.00	48.60	CH_4,H_2O, HDO
4290.40	56.80	CH_4, H_2O, HDO

The NDACC data product contains total columns, these could be converted to xCO values (column-averaged dry air volume mixing ratio of CO) using the measured surface pressure and H_2O total column (both are included in the GEOMS HDF files) to reduce systematic errors.
The official data product of TCCON is given as xCO which is obtained from total columns using the O_2 total column to reduce systematic errors.
In the official TCCON data product an additional correction of 0.6 percent is added to the retrieved data as a result of comparisons with in situ measurements. In the comparisons in the present study, total columns are compared and the latter corrections are not taken into account; but taking xCO would not change the general conclusions.

3. Results

3.1. Bremen FTIR station

Comparing the Bremen CO data (Fig. 1) one finds a very good agreement as to the shape of the seasonal cycle. The minima in August to September also show a very good agreement in retrieved values, while the maxima are slightly higher in the NDACC retrievals. The mean NDACC value is ~5% higher than the mean TCCON value. In Fig. 2 a scatter-plot for the Bremen site is shown, where retrieved values from both networks taken within 30 minutes of each other are compared. This shows clearly that the lower values of ~ $1.6*10^{18}$ molecules are in perfect agreement, while the NDACC retrieval is more sensitive to higher values.

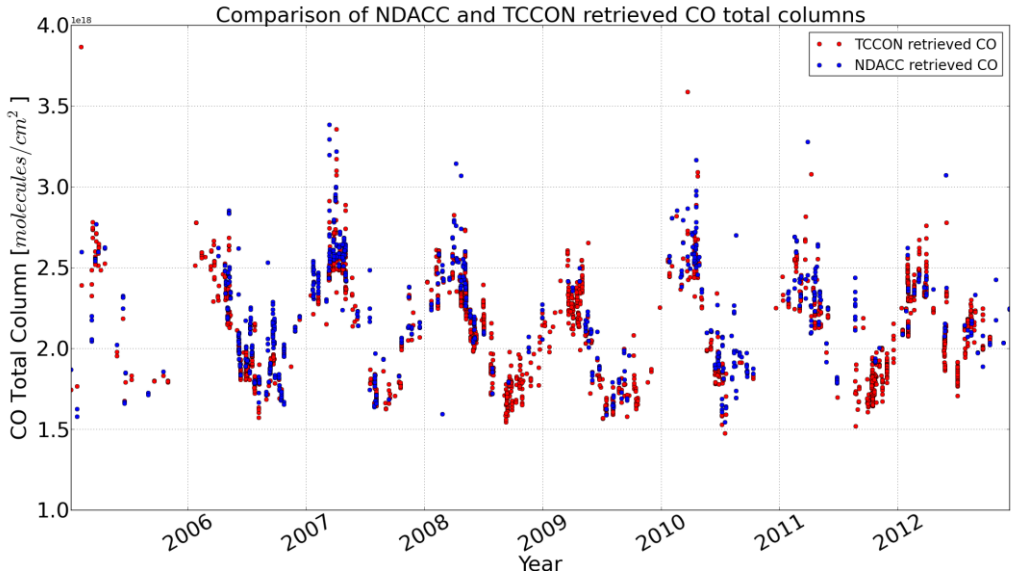

Fig. 1: CO columns as recorded at Bremen station.

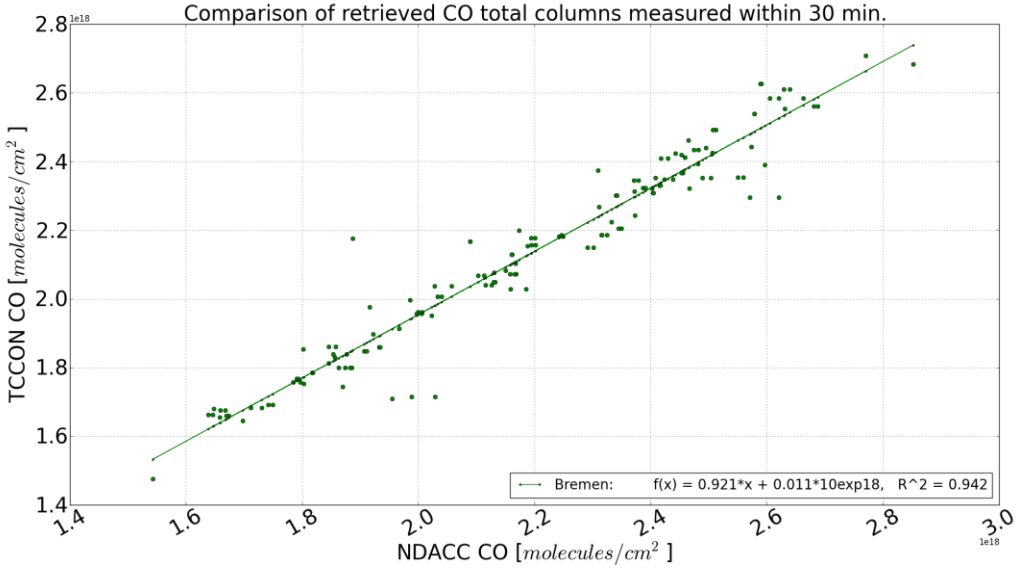

Fig. 2: Comparison of CO columns recorded at Bremen from NDACC and TCCON.

3.2. Izana Observatory

For the NDACC (MIR) analysis, the PROFFIT retrieval software has been applied. The software performs profile retrieval. The retrieval is performed in the log-VMR space, as this improves the description of the a-priori probability-density function for a gas of significant variability (as e.g. CO or H_2O). The a-priori profile has been taken from the WACCM Ver. 6 runs, as recommended by NDACC.
For the MIR work, 4 MWs have been applied (derived from recommendations provided by C. Rinsland).

Table 3. Microwindows for CO as recommended by C.Rinsland.

Window [wavenumbers]	Width [wavenumbers]	Interfering gases
2057.50 - 2058.20	0.70	H2O, CO2, O3, N2O, OCS
2069.40 - 2069.90	0.50	H2O, CO2, O3, N2O, OCS
2140.40 - 2141.40	1.00	H2O, CO2, O3, N2O, OCS
2153.20 - 2160.00	6.80	H2O, CO2, O3, N2O, OCS

As can be seen in Fig. 3, the annual minima are in close agreement, whereas the maxima indicated by the MIR time series are slightly higher. As a result, the annual variability indicated by the MIR time series is slightly higher (by about 20%). Still, the overall agreement between both approaches is very satisfactory.

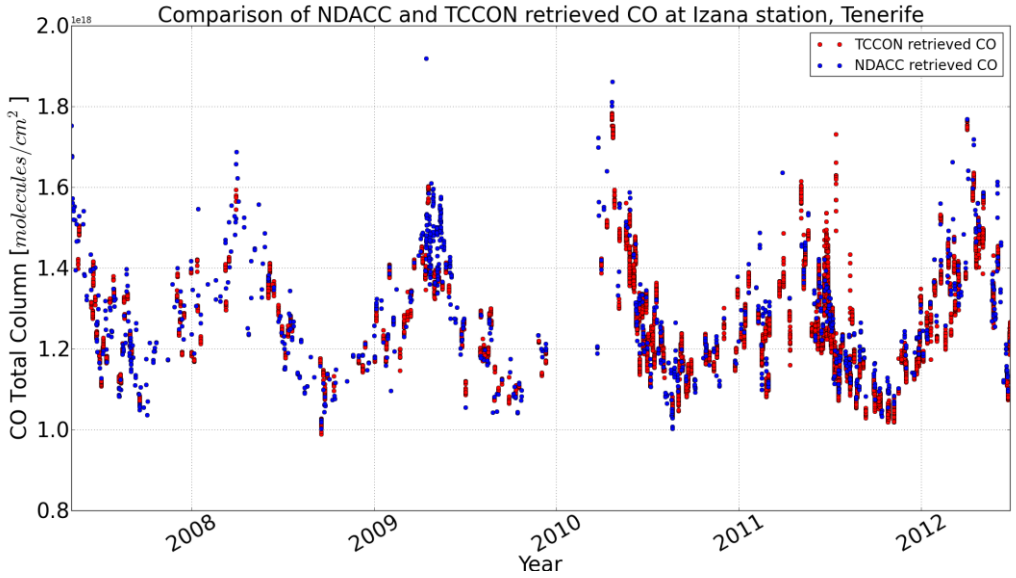

Fig. 3: CO columns as recorded at Izana observatory.

3.3. Jungfraujoch station

Recently a new FTIR retrieval strategy for CO has been tested at the Jungfraujoch station and the results have been compared with the CO strategy adopted for the NORS Rapid Data Delivery.
Currently NORS uses 3 microwindows in the 2000-2100 cm^{-1} wavenumber domain with WACCM v.6 as a priori model. As shown in Table 4, a CO retrieval in the 4200 cm^{-1} domain (recorded within the framework of NDACC commitments) has been investigated, using 5 microwindows and also WACCM v.6 as a priori. For both spectral regions, profile retrievals are performed with the SFIT-2 algorithm.

Table 4. 4200 cm^{-1} domain micro windows as investigated at Jungfraujoch.

Window [wavenumbers]	Width [wavenumbers]	Interfering gases
4209.20 - 4209.55	0.35	CO, CH4
4227.09 - 4227.80	0.71	CO, CH4
4231.47 - 4231.97	0.50	CO, CH4, HDO
4274.63 - 4274.965	0.335	CO, CH4, HDO
4284.82 - 4285.36	0.54	CO, CH4

Fig. 4 shows the CO total column retrieved from 1265 solar spectra at the Jungfraujoch according to the NORS strategy, compared to the results produced by the fitting of 670 spectra in the 4200 cm^{-1} domain for the 2010-2013 period. This reveals a good agreement between the two datasets. The investigated strategy generally gives higher DOFS (2.533 compared to 2.214 in average) and less residuals than the NDACC approach. For a full evaluation of the two strategies it is planned to compare only solar spectra registered approximately at the same time of the day for taking into account the CO intraday variability.

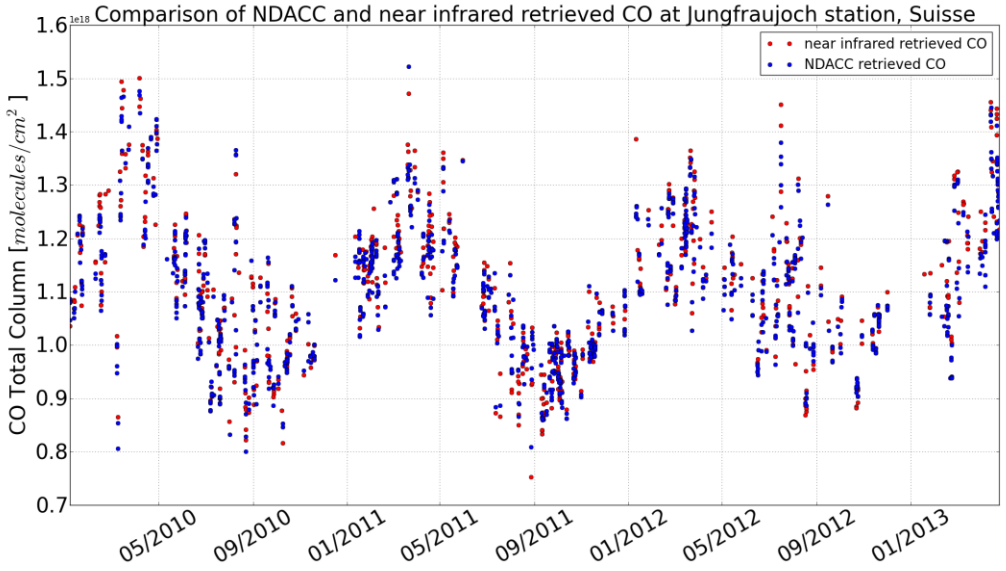

Fig. 4: CO columns as recorded at Jungfraujoch station.

3.4. St. Denis station, La Reunion

The measurement time period ranges from February 29 till September 4 in 2013 and represents total column values from both NDACC and TCCON measurements. There is a good correspondence between the TCCON and NDACC measurements, with a relative bias of

-2.5% in 2013; on average NDACC underestimates TCCON.
At La Reunion the NDACC retrieval strategy for CO is used. Both, NDACC and TCCON data products are generated by the same Bruker 125HR instrument at St. Denis.

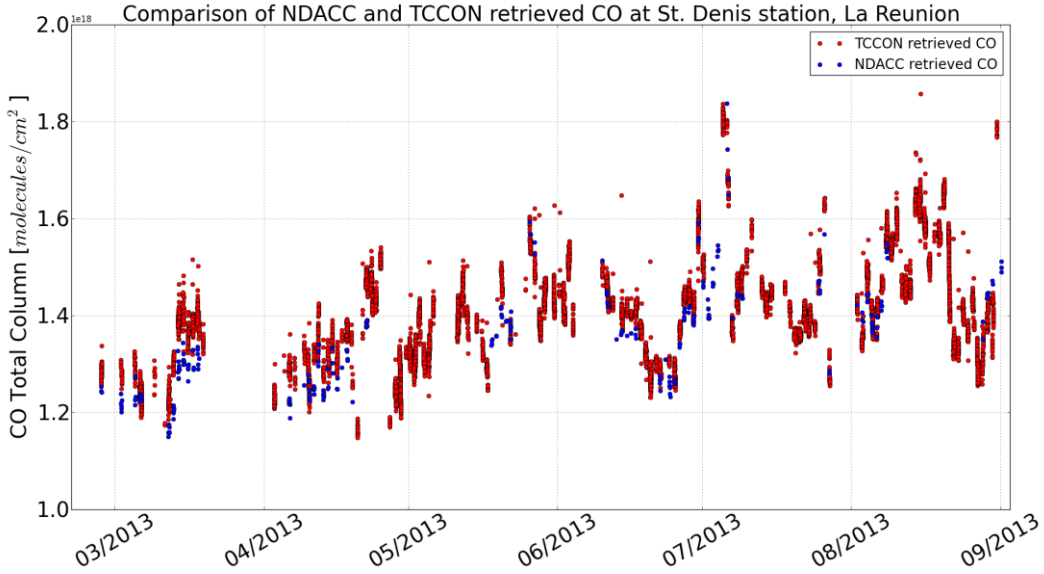

Fig. 5: CO columns as recorded at St. Denis station.

For St. Denis, the Averaging Kernels are shown. The coloured curves represent the calculated sensitivity for a special height in the concentration profile. The total column Averaging Kernel is the sum of the Averaging Kernels for individual heights. Having degree of freedom of 2.89 is a value for the number of height levels one could distinguish.

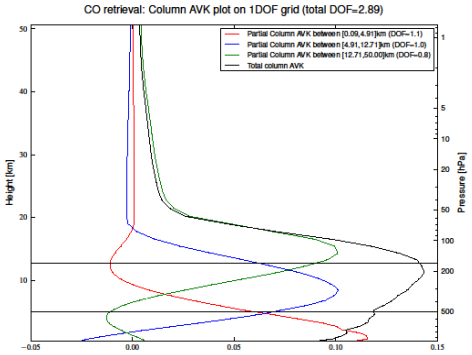

Fig. 6: Exemplarily the Averaging Kernels are shown for St. Denis station.

4. Conclusion

The relative differences for retrieved total columns from measurements recorded within 30 minutes from each other, comprising all contributing stations, shows a clear seasonal cycle. This cycle is shifted by 6 months for the St. Denis station, as it is situated in the southern hemisphere. The seasonal cycle of the relative difference is in-phase with the seasonal cycle of the total columns itself, indicating that the NDACC profile retrieval is more sensitive to concentration changes than the TCCON retrieval.

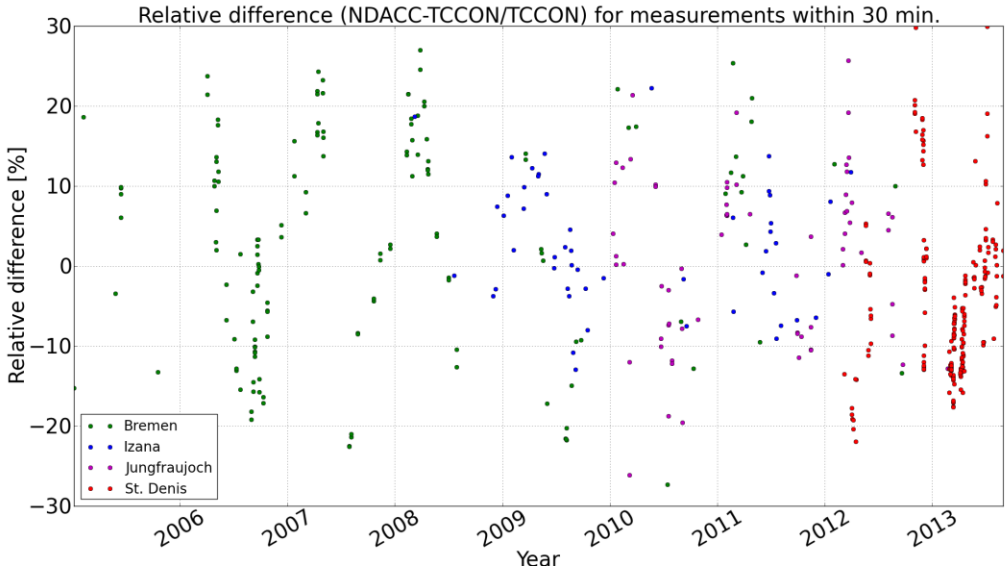

Fig. 7: Relative difference (NDACC-TCCON/TCCON spectral region) for the data sets from all contributing stations. Jungfraujoch station is not measuring TCCON standard but in the TCCON spectral region.

A scatter plot of the same data shows that the gradient of TCCON vs. NDACC is similar for Bremen, Izana and St. Denis.
Jungfraujoch station is measuring with NDACC standard in the mid infrared spectral region but not with TCCON standard in the near infrared spectral region. Comparing these retrieval strategies doing profile retrieval in both wavenumber domains shows a gradient of nearly one; this indicates good spectroscopic data for both wavenumber regions.

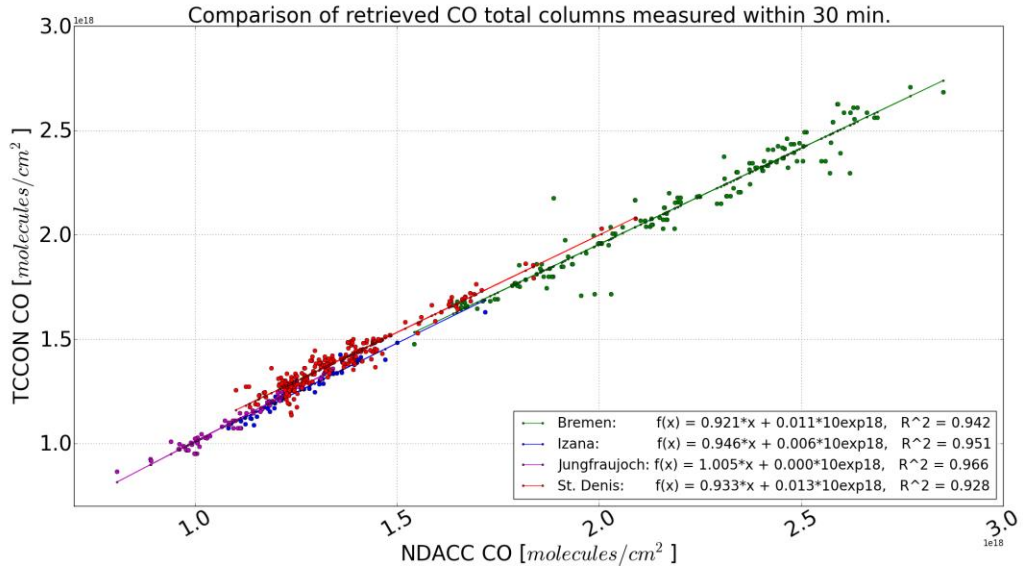

Fig. 8: Scatter plot with fitted slope for the data sets from all contributing stations. Jungfraujoch station is not measuring according to the TCCON standard but in the TCCON spectral region.

The overall agreement of the NDACC and the TCCON networks regarding the CO retrieval is satisfying but not perfect. The situation is different at the Jungfraujoch station for which two profile retrieval approaches are compared. The reason for the higher variability of NDACC vs. TCCON at the three other sites is assumed to be in the retrieval of the lower troposphere. NDACC is more sensitive to concentration variability and the concentration variability takes place mainly in the lower troposphere due to local influences. The profile retrieval therefore seems to have an advantage in being more flexible and less dependent on a priori input from external climatological data.