

FRM4GHG 2.0

Fiducial Reference Measurements for Greenhouse Gases



OCS retrieval from low-resolution spectrometers

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1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V0.0	2025-10-22	-	Initial version
V1.0	2025-11-13		Final version

2 ACCESS LIST

This document is a deliverable “D2.4.2 OCS retrieval from low-resolution spectrometers” created for the project FRM4GHG 2.0 CCN and will be submitted to ESA. The document can be downloaded from the project webpage <http://frm4ghg.aeronomie.be>.

3 PURPOSE

This document summarizes our first results on WP2: “D2.4.2 OCS retrieval from low-resolution spectrometers”. The objective is to demonstrate the feasibility of retrieving OCS from low-resolution spectrometers by using spectra from high resolution 125HR instruments and low resolution measurements of the Vertex70/Invenio.

4 DOCUMENT STRUCTURE

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5 RESULTS

5.1 Introduction

Carbonyl Sulfide (OCS) which results mainly from various anthropogenic sources and also the oxidation of sulfur containing species is the most abundant sulfur containing compound in the atmosphere. OCS proved to be an important atmospheric species when researchers found that it is a good surrogate for CO₂ for tracking how much carbon is taken up by photosynthesis worldwide. This is because, like CO₂, OCS is taken up by plants but is not released by respiration (Campbell et al., 2017). Based on this, OCS measurements in Sodankylä using various techniques (high and low resolution FTIR and Aircores) were performed.

The retrieval procedure used in the OCS retrieval from high resolution spectra is described in (Sha et al., 2024 and Hannigan et al., 2022). The low resolution Vertex70 spectra however, showed some

scatter noise in the time series when using the same procedure. Therefore, the Norton Beer Strong apodization (Griffiths and de Haseth, 2007) was used instead of Boxcar (see section 3.3.1 of Sha et al., 2024). Additionally, slightly wider retrieval windows were utilized which reduced this scatter significantly. SNR deweighting to a value of 500 was also improved the overall intraday variability. The median total error coming from the Vertex70 measurement is about 4.2% and the one coming from FTS-125HR is about 6.2%.

The other parameters stayed the same for both retrievals. The parameters chosen are given in the following table.

Spectrometer	FTS-125HR	Vertex70 (LR)
Retrieval Code	SFIT4	
Micro-windows (cm ⁻¹)	2047.85–2048.24 2049.77–2050.18 2054.33–2054.67	2047.15–2048.24 2049.17–2050.18 2054.13–2054.97
Retrieved species	OCS and O ₃ : profiles CO ₂ , CO, H ₂ O, C ¹⁸ O ₂ , solar lines: columns	OCS and O ₃ : profiles CO ₂ , CO, H ₂ O, C ¹⁸ O ₂ , solar lines: columns
A priori profiles	Climatology from WACCM v7 (excluding H ₂ O) monthly means NCEP 6-hourly profiles for H ₂ O 2023	Climatology from WACCM v7 (excluding H ₂ O) monthly means NCEP 6-hourly profiles for HDO and H ₂ O
Pressure and temperature profiles	NCEP 6-hourly profiles	NCEP 6-hourly profiles
Spectroscopy	HITRAN2020	HITRAN2020
Regularization	Tikhonov L1	Tikhonov L1

Table 1: Parameters used for measurements using the Vertex70LR and IFS125HR

5.2 OCS results from the Vertex 70LR

In 2019 a campaign was carried out in Sodankylä to perform measurements using the Vertex70 FTIR spectrometer. The interferometer has a max optical path difference of 4.5 cm, corresponding to a resolution of 0.22 cm⁻¹. Unfortunately, the high resolution measurements by the IFS125HR from Sodankylä, did not cover the spectral range used in the retrieval of OCS, which regrettably would not allow a daily coincidences comparison. Therefore, a visual comparison of the results was performed against the Kiruna site, about 270 km apart. The time series shown in Figure 1 demonstrates a clear intraday variability as well as a seasonal trend, comparable to the results from the FTS-125HR Kiruna. The noticeable scatter observed in the Vertex70 OCS results has been reduced as best as possible, and improvements on the retrieval will be further performed in the future to produce the most optimal OCS results using the low resolution FTIR spectra.

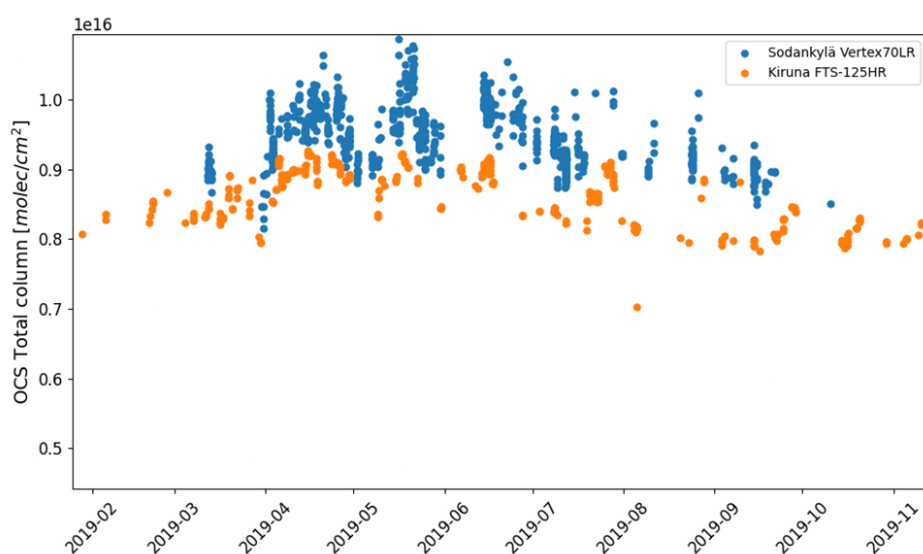


Figure 1: Time series of OCS retrieved from Vertex70 measurements from Sodankylä compared to OCS values from FTS-125HR in Kiruna. The median total error from the Vertex70 analysis was found to be about 4.2%.

5.3 Retrieval of OCS from FTS-125HR Sodankylä and comparison with Aircores

Three datasets were processed in this part. The results from the high resolution FTIR measurements in Kiruna and Sodankylä were compared to AirCore (AC) measurements that took place during a campaign in Sodankylä in 2023/08/02 and 2023/08/08, and in Kiruna in 2021/08/13 (two measurements for Kiruna one “wet” with no scrubber equipped and one “dry” with a scrubber). The OCS FTIR data for Kiruna were taken from the publicly available data on the NDACC website. The AC measurements from Sodankylä were missing some values at the boundaries and in the middle atmosphere. This might have caused the observed low values in the comparison to the spectroscopic measurements in Sodankylä.

The AirCore data were then smoothed with the average Averaging Kernels after re-gridding it to the FTIR height grid, using the equation 1.

$$X_{\{aircore\}} = X_{\{aircore\}} + A(X_{\{aircore\}} - X_{\{aircore\}}) \quad (1)$$

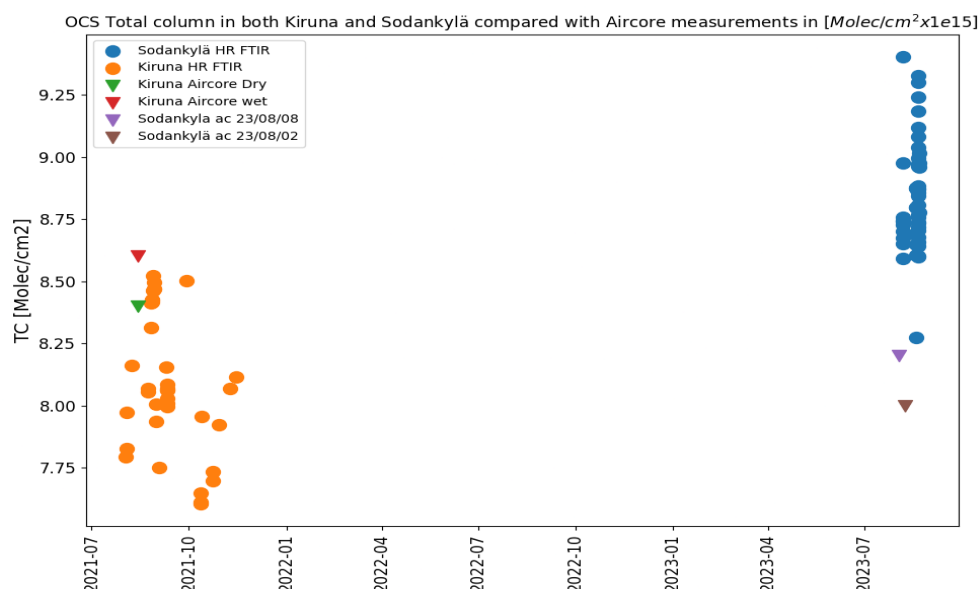


Figure 2: Comparison of high-resolution spectroscopic measurements of OCS at Sodankylä and Kiruna together with the AirCore data. The dry AirCore in Kiruna was equipped with a scrubber, the wet one was not. Both high resolution (HR) FTIR measurements from Kiruna and Sodankylä were performed using a Bruker IFS 125HR.

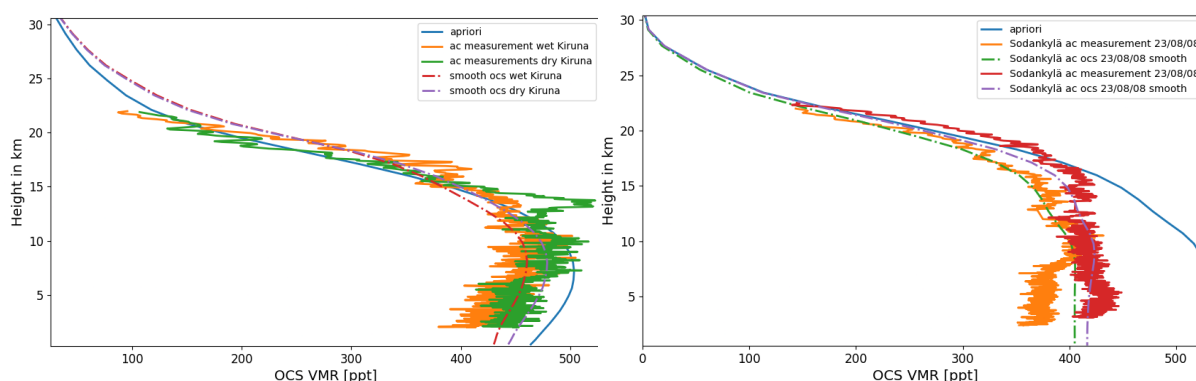


Figure 3: Comparison of a priori vmr profiles of OCS, used for the retrieval of the total column OCS, together with the vmr-profiles from the AirCore launches.

5.4 Summary

The low-resolution spectrometer allows to measure OCS with sufficient uncertainty. Unfortunately, no AirCore launches were performed at the times the low-resolution Vertex70HR was measuring but the comparison to the observations at Kiruna yield a reasonable agreement.

The comparison of OCS retrieved from the high-resolution measurements with the AirCore data in Sodankylä and Kiruna yield a sufficient agreement.

6 APPLICABLE DOCUMENTS

Statement of Work: Fiducial Reference Measurements for Ground-Based IR Greenhouse Gas Observations (FRM4GHG 2.0)
Prepared by: EOP-GMQ, Reference: ESA-EOPG-EOPGMQ-SOW-21

7 REFERENCE DOCUMENTS

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