Retrieval of total column densities of formaldehyde and sulphur dioxide from Sentinel-4 measurements

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Sulfur dioxide (SO_2)

SO_2 vertical column from S4

For SO_2, it is expected that S4 measurements will be able to detect low levels of anthropogenic SO_2 and improve on the existing satellite data sets due to the combination of high spatial resolution (8x8 km²) and high temporal sampling (1 hour). These aspects are also valuable in the monitoring of volcanic plumes.

At the same time, the geostationary observation geometry of S4 poses challenges to an SO_2 retrieval scheme that are not encountered with polar-orbiting sensors:

- Large viewing angles cause long light paths, leading to enhanced scattering and influence of ozone absorption.
- The changing illumination during the S4 scanning process implies changing photochemistry, requiring a new background correction scheme.
- Volcanic SO_2 plumes from Iceland will be situated at the northernmost edge of the S4 coverage area, where the largest observation angles occur.

The retrieval algorithm

The S4 bread-board algorithm for the retrieval of total SO_2 column is a DOAS[1]-type scheme based on algorithms for previous satellite sensors, such as S5P/TROPOMI (Theys *et al.*, 2017).
The full scheme, from S4 L1b radiance measurement to SO_2 vertical column, is depicted in Figure S-1.

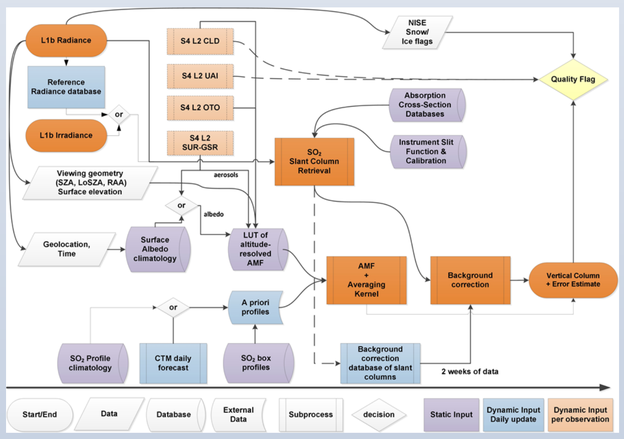

Figure S-1 Flow diagram of the S4 sulfur dioxide VCD retrieval algorithm.

The main steps are:

- Slant column density (SCD) fitting through a 3-window approach, accounting for possible saturation of the SO_2 signal for large SO_2 amount (like during volcanic eruptions). These windows are: 312-326 nm; 325-335 nm; 360-390 nm.
- Background correction of the SCD for residual SO_2 amounts that are usually found over clean areas or at large solar or viewing angle. This step involves a parameterization of the SO_2 residual as function of ozone slant column, based on a running average of measurements over two weeks.
- Determination of an airmass factor (AMF)
- Conversion of the SCD into a vertical column density (VCD)

The AMF calculation uses information from other S4 L2 products: cloud parameters (S4 L2 CLD), surface reflectance (S4 L2 SUR-GSR), and total ozone (S4 L2 OTO).

Application to test data

Retrieval tests on synthetic data (see "**Test data set**") show good results (retrieved column matches true VCD within 10-15% for SZA < 65°) for clear-sky scenarios without aerosols (Figure S-2).

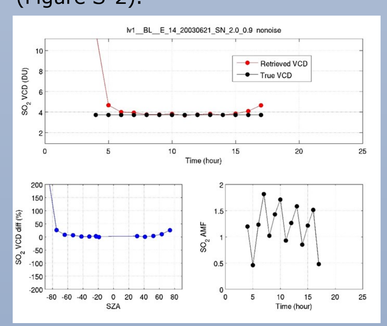

Figure S-2 SO_2 VCD retrieval performed on synthetic spectral data for Benkovski, Bulgaria, simulating the passage of an volcanic SO_2 cloud. Retrieved and true VCD agree with 10-15 %², except for the most extreme solar an-

As expected, the presence of aerosol impacts the retrieval accuracy (Figure S-3); The feasibility of applying aerosol correction schemes is under investigation.

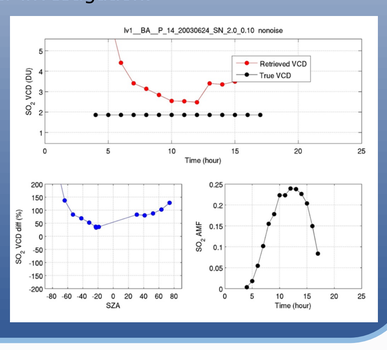

Figure S-3 SO_2 VCD retrieval performed on synthetic spectral data for a boundary SO_2 pollution scenario in Benkovski, with low optical depth aerosol in the morning and high optical depth in the afternoon. The aerosol presence clearly causes an offset in the retrieved SO_2 column.

Sentinel-4

Mission

Sentinel-4 is (S4) is a European Earth observation mission and part of the European Union Copernicus programme. The Sentinel-4 (S4) instruments will be launched on-board the MTG-S geostationary platforms, of which the first is scheduled for launch in 2023.

Observation geometry

The S4 instrument will observe the Earth's radiance within a geographic coverage area (GCA, blue contour in Figure 1) that includes Europe and North Africa. Most time of the nominal operations is spent in scanning the reference area (RA, green), hourly from east to west; the instant field of view (IFOV) of the 2D detector covers the full north-south extend of the coverage area. The remaining areas of the GCA, east and west of the RA, are scanned just after local sunrise and before local sunset, respectively. A typical scan pattern for a day of S4 observations is depicted in Figure 2.

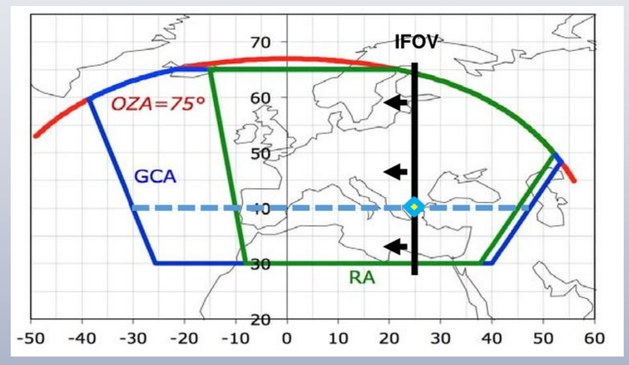

Figure 1 The observation area covered by Sentinel-4. The observation zenith angle (OZA) at the northernmost boundary is 75 degrees.

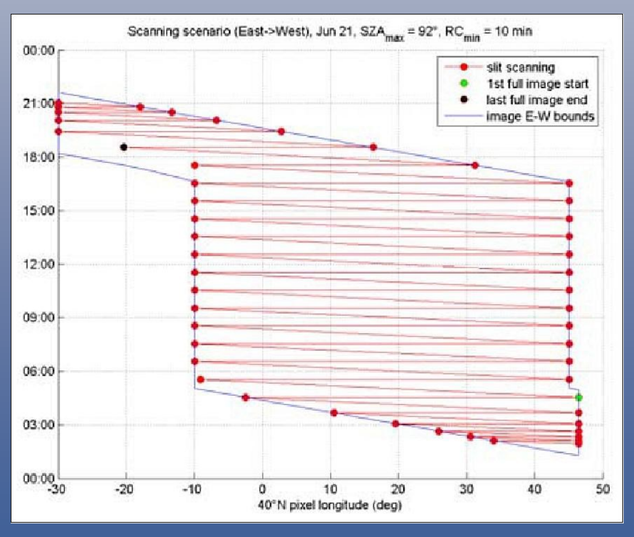

Figure 2 Typical east to west scan pattern of Sentinel-4.

The Sentinel-4 L2 project

The project *Sentinel-4 Level-2 Processor Component Development* (S4L2) is an activity for ESA, performed by a consortium of 8 European institutes and led by the German Aerospace Center (DLR). The project foresees in

- The development of bread-board retrieval algorithms for a range of atmospheric constituents.
- Independent verification of the prototype algorithms and the generation of test data sets for this purpose.
- The development and configuration of prototype and operational S4 L2 processors, implementing the bread-board algorithms.

BIRA-IASB is responsible for the development of the bread-board algorithms for the retrieval of total vertical columns of formaldehyde (HCHO) and sulfur dioxide (SO_2), is involved in the algorithm for total ozone, and will perform the independent verification of the glyoxal total column algorithm.

Test data set

For the S4 L2 project, the colleagues from MPIC Mains have generated a test data set (TDS) of synthetic spectra and atmospheres that is used by the bread-board L2 algorithms and the verification schemes. The TDS provides data for 17 different locations over Europe and incorporates physical aspects like cloud cover, aerosol presence and volcanic ash.

[1] Discrete Optical Absorption Spectroscopy

[2] Non-methane volatile organic compounds

Formaldehyde (HCHO)

HCHO vertical column from S4

The S4 mission is of high interest for HCHO observations because of the hourly repeat cycle. This allows for the study of the diurnal HCHO variation, which currently is poorly known, and therewith the quantitative derivation of NMVOC[2] emissions.

The geostationary observation geometry of S4 poses challenges to an HCHO retrieval scheme due to the changing scene illumination and long light path lengths. This implies changing chemistry and enhances the effect of aerosol presence and 3D cloud effects. For polar orbiting sensors, clean areas over the Pacific are normally used for background correction. For S4, an alternative approach needs to be found for this, as it only scans the Atlantic at the end of the day.

The retrieval algorithm

The S4 bread-board algorithm for the retrieval of total SO_2 column is a DOAS[1]-type scheme based on algorithms for previous satellite sensors, such as S5P/TROPOMI (De Smedt *et al.*, 2018).
The full scheme, from S4 L1b radiance measurement to SO_2 vertical column, is depicted in Figure H-1.

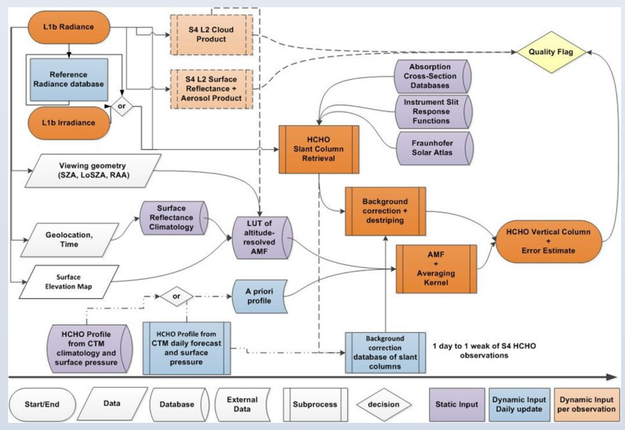

Figure H-1 Flow diagram of the S4 formaldehyde VCD retrieval algorithm.

The main steps are:

- Derivation of slant column density (SCD) from the S4 L1b spectrum. The SCD fitting is done in two steps:
  1. BrO pre-fit in the 328.5-359 nm window: This interval includes six BrO absorption bands and minimizes the correlation with HCHO.
  2. HCHO SCD retrieval in the 328.5-346 nm window, using the BrO values determined in the first step.
- A background correction to account for residual, latitude-dependent biases in the HCHO SCD as well as for striping that may occur due to imperfect cross-calibration of the different S4 detector rows. The use of clean regions over the Pacific is out of scope for S4 and alternative approaches are under investigation, such as the use of a dependency on ozone columns as used for the SO_2 product. For tests performed on synthetic spectral data, so far an Atlantic region, combined with a parameterization as function of solar zenith angle has been used.
- Determination of an air mass factor (AMF)
- Conversion of the SCD into a vertical column density (VCD)

The AMF calculation uses information from other S4 L2 products: cloud parameters (S4 L2 CLD) and surface reflectance (S4 L2 SUR-GSR).

Application to test data

Test retrievals have been performed on the TDS (See "**Test Data Set**"). Boundary layer aerosol affects the retrieved column value by 10-100%, depending on distribution and optical depth (Figure H-2).

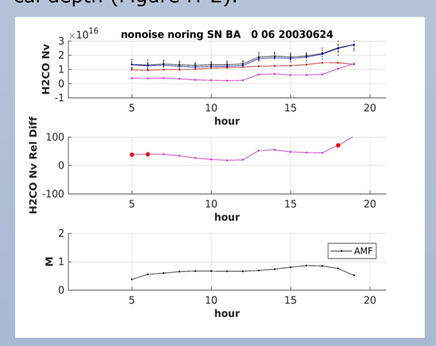

Figure H-2 Retrieval of HCHO VCD (N_V) from synthetic data over Milan. Boundary layer aerosol optical depth is low in the morning and high in the afternoon.

The colors in the top panel represent:

True column
Retrieved column
Background corrected retrieved column
Difference

When not accounted for, the presence of cloud can severely affect the retrieved HCHO column (Figure H-3).

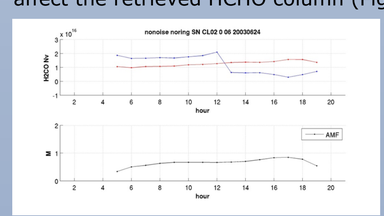

Figure H-3 The effect of partial cloud cover (Milan), when this is not taken into account in the AMF calculation.

True column
Retrieved column

First tests show this can be corrected for by using cloud parameters obtained from the S4 L2 CLD algorithm in the AMF calculation (Figure H-4).

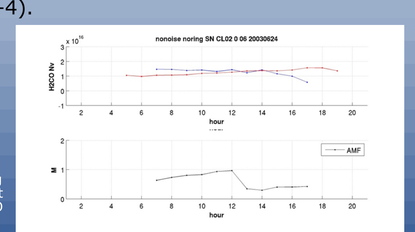

Figure H-4 When taking the cloud cover into account in the AMF, the derived HCHO column improves.