TOTAL COLUMN RETRIEVAL OF SO_2 AND HCHO FROM SENTINEL-4 MEASUREMENTS

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ABSTRACT

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 2024. BIRA-IASB is responsible for the development of bread-board algorithms for the retrieval of total vertical column quantities of sulfur dioxide (SO_2) and formaldehyde (HCHO). Tests of these algorithms on synthetic S4-spectra show that the SO_2 and HCHO algorithms are capable of retrieving the vertical column with an uncertainty of 10-15% for solar zenith angles smaller than 65 degrees, under clear-sky conditions and without the presence of aerosol.

Index Terms— Sentinel, S4, atmospheric chemistry, sulfur dioxide, formaldehyde

1. INTRODUCTION

Sentinel-4 is the first geostationary mission in the series of Earth observing Sentinel-platforms within the Copernicus programme of the European Union. Also, it is the first European geostationary mission dedicated to the monitoring of atmospheric chemistry and composition. S4 will observe the European domain and part of northern Africa, with a spatial resolution as fine as 8x8 km² (ground pixel size). The geostationary position allows S4 to measure with a revisit time of one hour, allowing the detection of diurnal variation of atmospheric trace gas quantities and the monitoring of transport (e.g. volcanic plumes). Other geostationary atmospheric composition missions are TEMPO (observing North America, launch 2020) and GEMS (monitoring East Asia, 2020).

The project *Sentinel-4 Level-2 Processor Component Development* (S4L2) is an activity for the European Space Agency ESA, performed by a consortium of eight European institutes and led by the German Aero-space Center (DLR). The project foresees in 1) The development of bread-board retrieval algorithms for a range of atmospheric constituents; 2) Independent verification of these algorithms and the generation of test data sets for this purpose; 3) 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). In addition, BIRA_IASB is involved in the algorithm for total ozone, and will perform the independent verification of the glyoxal total column algorithm.

The S4 mission is of high interest for HCHO observations be-cause of the hourly repeat cycle. This allows for the study of the diurnal HCHO variation, which currently is poorly known; this subsequently allows the quantitative derivation of emissions of non-methane volatile organic compounds (NMVOC), of which formaldehyde is a decay product. At BIRA-IASB, long standing experience exists with the retrieval of HCHO columns from satellite measurements ([1], [2], [3]).

For SO_2, it is expected that S4 measurements will improve on existing satellite data sets due to the combination of S4's high spatial resolution and high temporal sampling (1 hour). These aspects are also valuable in the monitoring of volcanic plumes. BIRA-IASB has many years of experience in retrieval studies and algorithm development related to SO_2 measurements from polar orbiting sensors [5], [6], [7]. The SO_2 retrieval algorithm presented in this paper builds on this experience.

1.1 Observation geometry

The S4 instrument will observe the Earth's back-scattered 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

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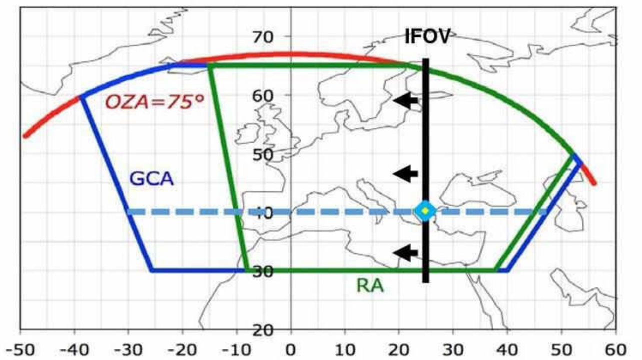

Figure 1. The observation area covered by Sentinel-4. The observation zenith angle (OZA) at the northernmost boundary is 75 degrees.

in Figure 2.

1.2 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.

2. SULFUR DIOXIDE

As mentioned before, S4 will allow the detection of low levels of anthropogenic SO_2. On the other hand, the geostationary observation geometry also poses some challenges not encountered with polar-orbiting sensors:
1) Large viewing angles cause long light paths, leading to enhanced scattering and influence of ozone absorption; 2) The changing illumination during the S4 scanning process

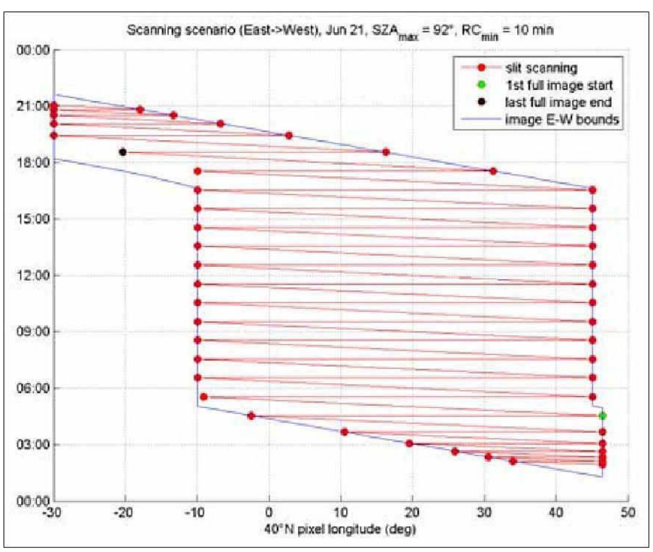

Figure 2. Typical east to west scan pattern of Sentinel-4 (source: ESA)

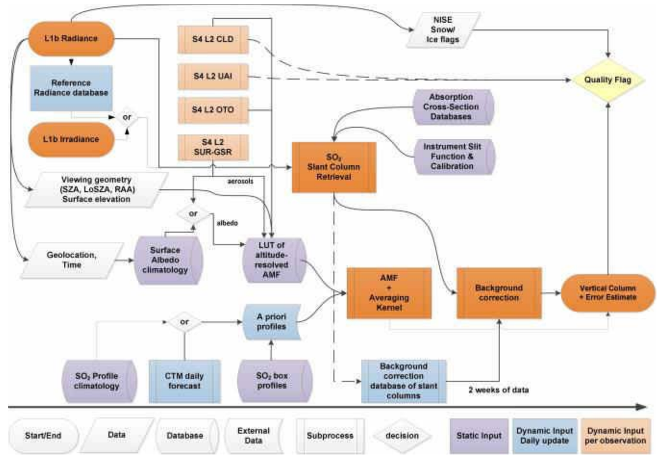

Figure 3. Flow diagram of the S4 sulfur dioxide VCD retrieval algorithm.

implies changing photochemistry, requiring a new background correction scheme; 3) Volcanic SO_2 plumes from Iceland will be situated at the northernmost edge of the S4 coverage area, where the largest observation angles occur.

2.1 The retrieval algorithm

The S4 algorithm for the retrieval of total SO_2 column is based on the principle of Discrete Optical Absorption Spectroscopy (DOAS, [8]). The algorithm builds on algorithms for previous satellite sensors, such as S5P/TROPOMI [2]. The full scheme is depicted in Figure 3. The main processing steps are:

1. 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.
2. 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.
3. Determination of an air-mass factor (AMF)
4. Conversion of the SCD into a vertical column density (VCD)

In its final version, the AMF calculation will use information from other S4 L2 products: cloud parameters (S4 L2 CLD), surface reflectance (S4 L2 SUR-GSR), and total ozone (S4 L2 OTO).

2.2 Tests on synthetic spectral data

Using the synthetic spectra described in section 2.1, the SO_2 algorithm was tested by retrieving the SO_2 VCD from the spectra for all 17 test locations. In the algorithm, several correction settings for the presence of clouds where applied;

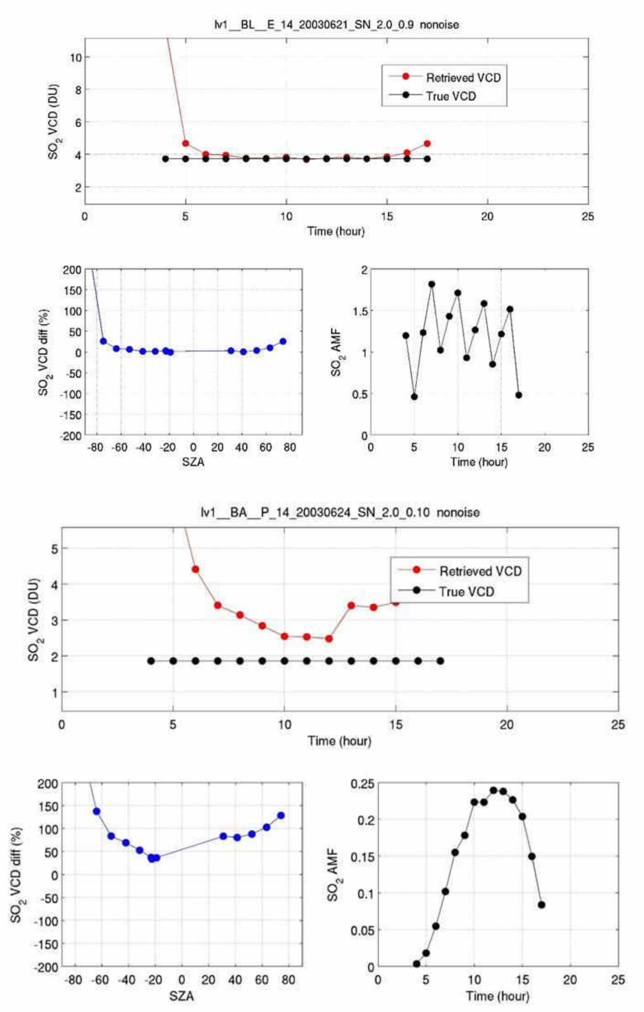

Figure 4. Synthetic SO_2 retrieval results over Benkovski, Bulgaria.

Aersols in the scene have so far been ignored by the algorithm. An example of retrieved VCD is given in Figure 4 for the location of Benkovski, Bulgaria. The top panel shows retrieval results for the passage of a volcanic SO_2 cloud. The retrieved VCD (red) agrees well with the true column (black), within 10-15%, for SZA < 65°. Large errors are found for large solar angles. These results are typical for the encountered cloud-/aerosol-free scenes. The bottom panels show a scenario of boundary layer SO_2 content and with aerosol presence in the atmosphere (low and high aerosol optical depth in the morning and afternoon, respectively). As can be expected, the deviation of the retrieved SO_2 column from the truth is now much larger. The application of aerosol correction schemes are not straightforward, but are subject of current investigation. In operational retrieval circumstances, cloud cover correction will be applied with aid of parameters obtained by the S4 L2 CLD algorithm.

3. FORMALDEHYDE

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 and the quantitative derivation of NMVOC 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 part the Atlantic at the end of the day. The S4 background correction scheme is still under development.

3.1 The retrieval algorithm

The HCHO algorithm is a DOAS-type scheme based on algorithms for previous satellite sensors, such as S5P/TROPOMI ([1]). The full scheme is depicted in Figure 4. The main steps are:

1. Derivation of slant column density (SCD). The SCD fitting is done in two steps: 1) BrO pre-fit in the 328.5-359 nm window: This interval includes 6 BrO absorption bands and minimizes the correlation with HCHO; 2) HCHO SCD retrieval in the 328.5-346 nm window.
2. 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. Tests with OMI data over the S4 domain look promising and will be further refined in the near future.
3. Determination of an air mass factor (AMF).
4. Conversion of the SCD into a vertical column density.

In its final version, the AMF calculation will use information from other S4 L2 products: cloud parameters (S4 L2 CLD)

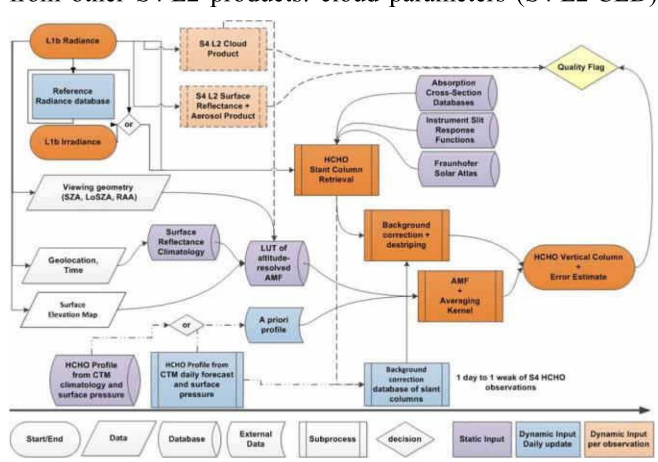

Figure 5. Flow diagram of the S4 formaldehyde VCD retrieval algorithm.

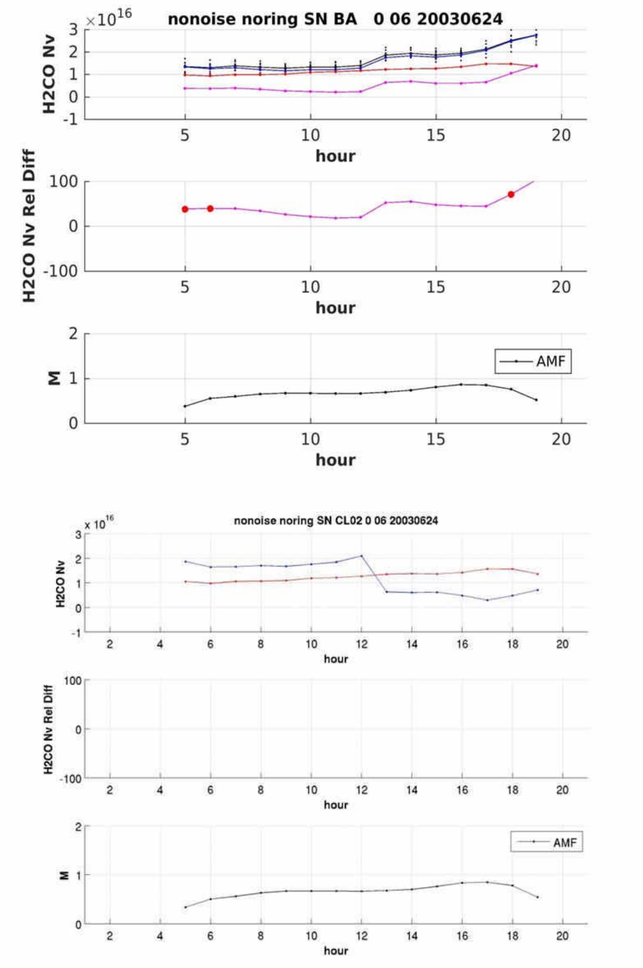

Figure 6. Synthetic HCHO retrievals over Milan.

and surface reflectance (S4 L2 SUR-GSR).

3.2 Tests on synthetic spectral data

Also for HCHO, tests on the synthetic spectra have been performed. Figure 5 shows an example of HCHO VCD retrieval from synthetic spectra over Milan, Italy. This scenario has low boundary layer aerosol optical depth in the morning and high in the afternoon. Despite the presence of aerosol, the retrieved HCHO VCD agrees with the true value within 10-100%. The impact of cloud cover (bottom panel) has a relatively large impact.

4. SUMMARY

Sentinel 4 is a future European mission for the geostationary monitoring of atmospheric composition over the European and northern African domain. Within the S4L2 project, BIRA-IASB is responsible for the development of the bread-board algorithms for S4 total column retrieval of sulfur dioxide and formaldehyde. Tests of the algorithms on synthetic spectra show a typical agreement between retrieved and true VCD of 10-15% for SO_2 and 10-100% for formaldehyde in the absence of clouds and aerosol. Depending on the exact scenario, clouds and aerosol can lead to much larger errors and tests where these phenomena are taken into account are currently ongoing.

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