Retrieval of formaldehyde from GEMS in preparation of the geostationary Sentinel-4 mission.

J. van Gent[1], I. De Smedt[1], H. Yu[1], C. Fayt[1], C. Lerot[1], N. Theys[1], D. Loyola[2], R. Lutz[2], R. Park[3], H.-A. Kwon[4], G. Lee[3], C. S. Lee[5], M. Van Roozendael[1], and the S4-L2 team.

[1] Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Brussels, Belgium; [2] Institut für Methodik der Fernerkundung (IMF), Deutsches Zentrum für Luft und Raumfahrt (DLR), Oberpfaffenhofen, Germany; [3] Seoul National University, Seoul, South Korea; [4] Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, United States; [5] National Institute of Environmental Research, Incheon, South Korea

Contact:
Jeroen.vangent@aeronomie.be
BIRA-IASB
3 Avenue Circulaire
1180 Brussels
Belgium
uvvis.aeronomie.be

The Sentinel-4 mission

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 2024.

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.

The ground pixel size for the S4 measurements will be as small as 8x8 km^2.

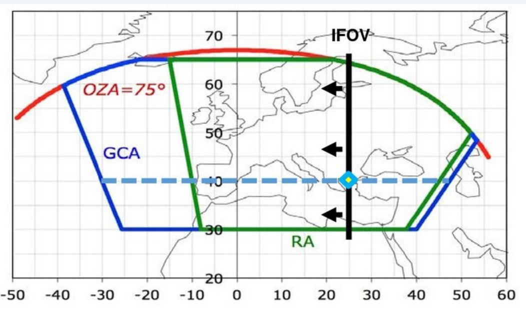

Figure 1 The observation area covered by Sentinel-4. The observation zenith angle (OZA) at the northernmost boundary is 75 degrees.

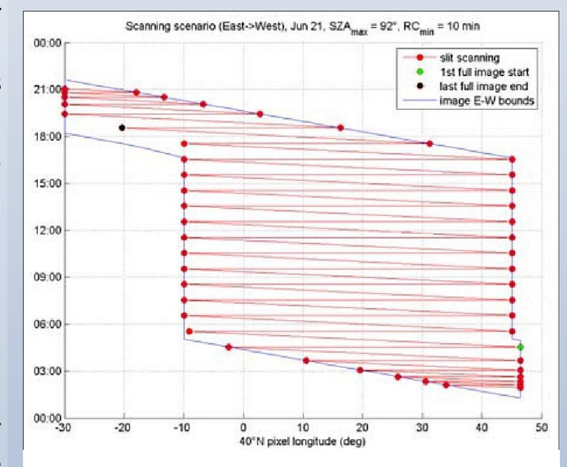

Figure 2 Typical east to west scan pattern of Sentinel-4.

The S4L2 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. **See also talk 1.3.3.**

S4 Formaldehyde retrieval

The S4 mission is of high interest for HCHO observations because of the hourly repeat cycle. This allows for the study of the diurnal variation of HCHO, 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 paths (Figure 3). 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.

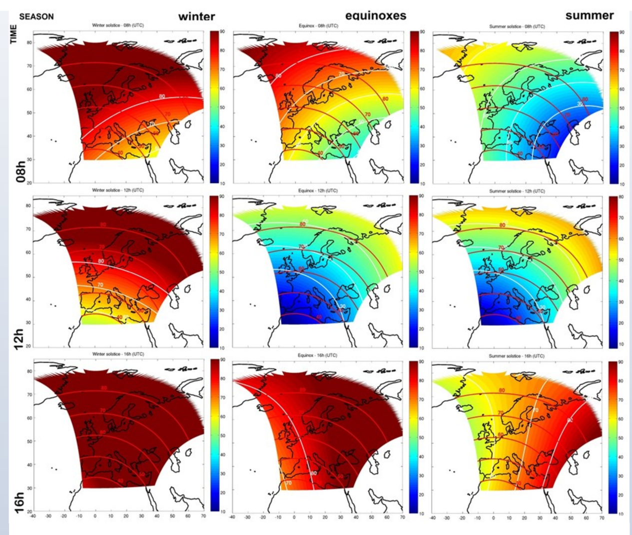

Figure 3 Solar zenith angles (color-coded) over the S4 observation domain at 8, 12, 16 h UTC (lines) at winter solstice (left panels), equinoxes (centre panels) and summer solstice (right panels). The red and white curves are viewing zenith angle and solar zenith angle iso-lines, respectively. Data have been provided through the courtesy of ESA.

The S4 bread-board algorithm for the retrieval of total HCHO column is a DOAS[1]-type scheme based on algorithms for previous satellite sensors, such as S-5P/TROPOMI (De Smedt *et al.*, 2018[3]). As is the case with polar sensors, the application to S4 measurements is expected to show large offsets and striping patterns, due to imperfect slant-column fits and instrumental characteristics. For polar orbiting instruments, these phenomena are usually corrected by means of a background correction step. This involves a reference region over the Pacific ocean, where the formaldehyde columns are small and well known. The S4 observation domain unfortunately does not cover any remote oceanic regions.

Within the frame of the ESA S4L2 project (see talk 1.3.3), the HCHO retrieval scheme has been tested and improved by using synthetic spectral data over 17 discreet locations in the S4 observation domain. Although this is highly useful, spectral data covering the full S4 frame are lacking, preventing the search for suitable techniques for background correction and destriping.

By using GEMS data, ideas can be developed and tested for destriping and offset correction. It is expected that these can then be applied to S4 data and fine-tuned after the launch of S4.

GEMS

Mission

The Geostationary Environment Monitoring Spectrometer (GEMS), launched on-board the GEO-KOMPSAT-2B satellite in February 2020 is the first geostationary sensor dedicated to air quality and atmospheric composition measurements. GEMS (observing South-East Asia hourly) will be joined by TEMPO in 2022 (United States) and Sentinel-4 (S4, 2024), monitoring Europe and Northern Africa.

Spectral response function (SRF)

Analysis of the spectral response function of GEMS (SRF, slit function) shows highly symmetrical profiles, with very small dependence on the detector rows. When optimizing the SRF in the BIRA-IASB QDOAS retrieval software, deviations from the key data are small, with indication of some small degradation after launch for wavelengths below 375 nm. All in all, the homogeneity of the SRF indicates high-quality instrumental optics.

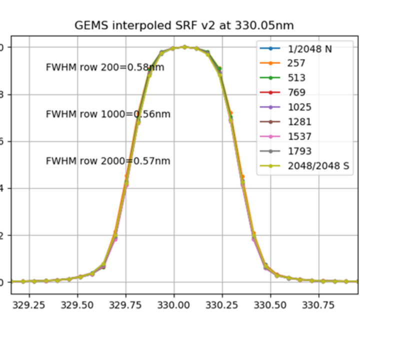

Figure 4 GEMS slit function profile from the GEMS key data for as central wavelength of 330.05 nm. The different profiles represent the different across-scan detector rows. Similar homogeneous profiles are observed at other wavelengths.

Wavelength calibration

By using a SAO high resolution solar atlas, wavelength shift up to 0.1 nm are observed in the GEMS irradiance spectrum. Furthermore, the shifts evolve over time (not shown), indicating the need to use daily irradiance spectra in the HCHO retrieval. After wavelength calibration, remaining shifts <0.03 are seen in the radiance spectra. Investigation into the interdependency of the different shifts is ongoing.

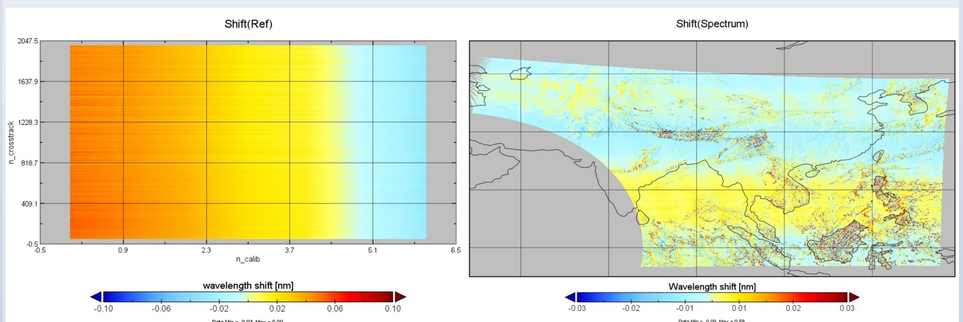

Figure 5 Example of observed GEMS irradiance wavelength shifts s function of wavelength and detector row (left) and remaining wavelength shifts in radiance after calibration (right). The depicted data is for 21 March 2021.

Slant column retrieval

In the HCHO DOAS retrieval from GEMS, so far the focus has been on slant column density (SCD) retrieval and prliminary background correction. Air mass factor related aspects will be studied later.

The applied retrieval configuration is as follows:

- Wavelength calibration
- Use of daily irradiance spectrum as reference
- Fitting window: 328.5-359 nm
- Cross sections: HCHO, BrO , NO2, O_4, O_3 (223 K+243 K, with I0 correction), O_3 "Pukite" terms, Ring effect
- 5th order polynomial
- Fitting of radiance shift and stretch and a linear offset

First results (example in Figure 6) are very promising, and oberved background offsets are relatively small, showing the high quality of the spectral measurements. But some artefacts are still observed: increased fit residuals (RMS) are visible over mountains and clouds and along coastlines (Figure 6, left panel). And, as for other 2D-detectors, a striping pattern is oberved in the raw SCD values (middle panel). A first, rudimentary destriping attempt was devised, by:

- removing pixels with RMS > 3e-3 (bad observations).
- Removing SCD values larger than twice the standard deviation, per row (possible real, elevated HCHO columns).
- Subtracting the median SCD value, per row, from the retrieved SCD values.

For this, the whole observation domain, rather than a dedicated reference sector was used. Still, this simple destriping mechanism appears to serve well as an SCD background correction step (right panel).

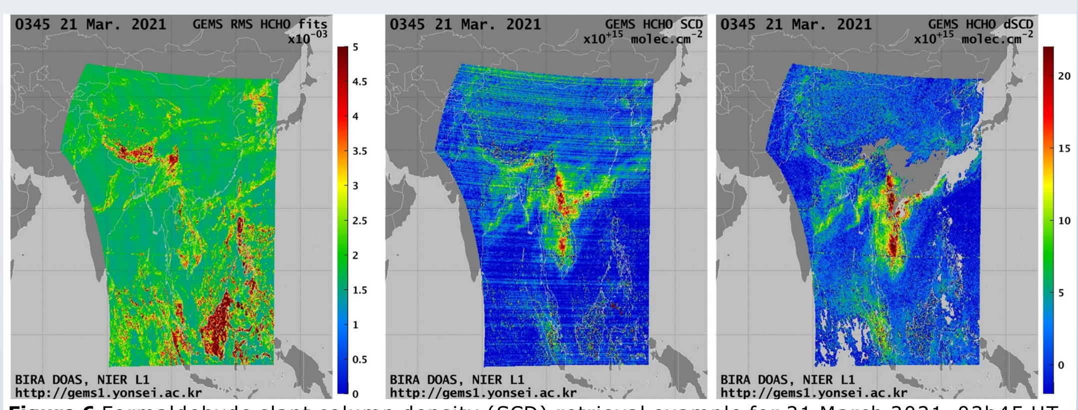

Figure 6 Formaldehyde slant column density (SCD) retrieval example for 21 March 2021, 03h45 UT. The panels represent fit RMS (left), uncorrected SCD (middle), and destriped SCD (right).

Diurnal variation

When considering HCHO retrieval, one of the most interesting aspects of a geostationary mission is the capability to observe the diurnal variation of the formaldehyde quantities. Initial SCD results for succesive hourly observations showed increasingly degraded fits towards the afternoon, in particular in the southern regions of the scene (example in Figure 7). This was also observed in data from the operational GEMS HCHO algorithm (a direct fitting scheme, results not shown here). As an attempt to remedy this, parameters describing the instrument's polarization sensitivity where obtained and included in the fitting procedure as a pseudo-absorber. This strongly improves the results, as can be seen in Figure 8. Interestingly, the highest HCHO columns are observed in the morning. Elevated columns values along the coastlines may indicate the effect of heterogeneous scenes, requiring more investigation.

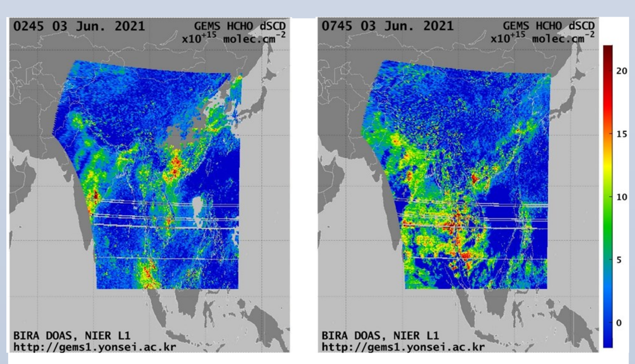

Figure 7 3 June 2021. Example of destriped morning and afternoon HCHO slant column results when ignoring the instrument sensitivity to polarisation. The fit quality clearly deteriorates in the afternoon.

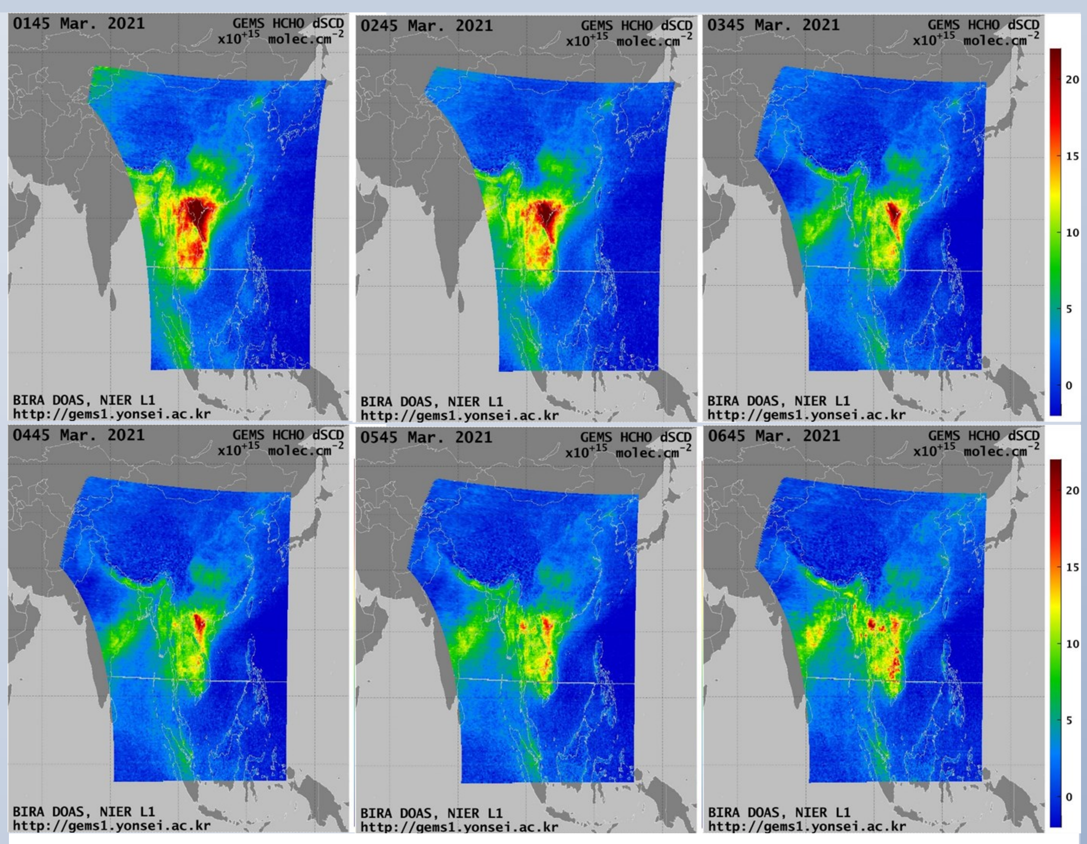

Figure 8 Ten-day average of retrieved formaldehyde slant columns for March 2021, after destriping and accounting for polarisation sensitivity in the fit. The fit quality over the day is rather consistent. Coastal lines often show elevated formaldehyde columns, possibly as a results of scene heterogeneity.

GEMS—TROPOMI comparison

First comparisons of GEMS DOAS slant column results with those from the well-established S-5P/TROPOMI DOAS algorithm show good agreement, with the GEMS values being somewhat lower than those from TROPOMI (Figure 9). The two instruments agree well in showing the seasonal variation (not shown here). Further refinement of the GEMS algorithm will likely show even better agreement in the future.

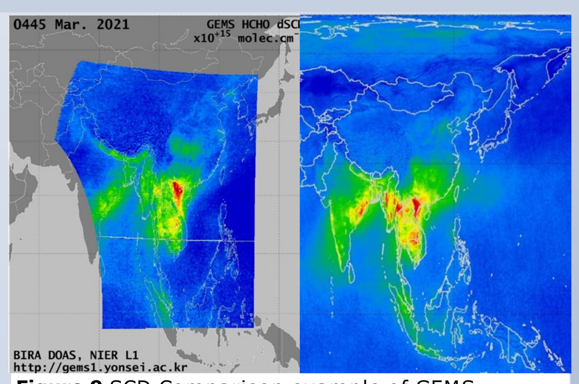

Figure 9 SCD Comparison example of GEMS (destriped 10-day average, left) vs. TROPOMI (mostly average) for March 2021.

Summary

The first analysis of GEMS spectra and formaldehyde SCD retrieval shows an instrument with fine optical characteristics, producing high quality spectra. Observed offsets on uncorrected slant columns are low, and first attempt at destriping has been shown to work well; the use of daily irradiance spectra as reference may be sufficient for this instrument. Ideally this would eliminate the need for advanced methods like the use of radiance spectra as reference, which is challenging by lack of remote oceanic surfaces in the scene. Knowledge of the polarisation sensitivity was found to be crucial and the effect of heterogeneous scenes needs further investigation.

The GEMS results are a promising first step towards optimization of formaldehyde retrieval from Sentinel-4. However, formaldehyde columns within the S4 domain are typically much lower, viewing angles are larger, and also the S4 instrument is known to be sensitive to polarisation and scene heterogeneity. Extensive further investigation is necessary to refine the retrieval settings and background correction details of the S4 HCHO algorithm.

GEMS data used for this poster were provided by NIER for validation and improvement research purposes as part of support for AO activities.

[1] Discrete Optical Absorption Spectroscopy; [2] Non-methane volatile organic compounds;

[3] De Smedt et al., Algorithm theoretical baseline for formaldehyde retrievals from S5P TROPOMI and from the QA4ECV project, Atmos. Meas. Tech., 11, 2395–2426, https://doi.org/10.5194/amt-11-2395-2018, 2018.

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