New Developments in the SCIAMACHY L2 Ground Processor

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Introduction

The SCIAMACHY Quality Working Group (SQWG) was founded in 2007 to improve the quality of the existing products and to implement retrievals of new data products. The SQWG consists of the experts from University of Bremen (lead), Belgian Institute for Space Aeronomy (BIRA), Remote Sensing Technology Institute at German Aerospace Center (IMF-DLR), Netherlands Institute for Space Research (SRON) and Royal Netherlands Meteorological Institute (KNMI).

The Version 6 of the L1b-2 processor has been delivered to ESA and become operational. The public release, after validation, is planned for the end of 2016.
Currently the SQWG Level 2 team is working on the Version 7 of the L1b-2 processor. In this version major improvements will be tropospheric BrO product, updated limb cloud detection scheme. In addition the new version is planned for release in a new future-proof file format based on NetCDF.

SCIAMACHY Instrument

- Spectrometer SCIAMACHY on-board ENVISAT
- Measurements between August 2002 and April 2012
- Wavelength range: 8 channels ranging from UV/VIS to NIR
- Two main observation geometries:
  - Nadir mode: observing the atmospheric volume directly under the instrument
  - Limb mode: the instrument looks at the edge of the atmosphere
- List of products (L2 Version 6):

Nadir Products	Glyoxal (CHOCHO)
Absorbing Aerosol Index	Water vapour (H_2O)
Ozone total column	Carbon monoxide (CO)
Nitrogen dioxide (NO_2)	Methane (CH_4)
Tropospheric NO_2	Cloud parameters (fraction, top height, optical density)
Bromine monoxide (BrO)	**Limb Products**
Tropospheric BrO (planned for L2v7)	Ozone profiles
Sulphur dioxide (SO_2)	NO_2 profiles
Chlorine dioxide (OClO)	BrO profiles
Formaldehyde (HCHO)	Limb clouds

Tropospheric *BrO* product

The retrieval based on the scientific algorithm developed at BIRA[1]. The main principle of the new algorithm is to utilize ***BrO*** total columns (already an operational product, DOAS fit window 336–351 nm) and split them into stratospheric $\boldsymbol{VCD_{strat}}$ and tropospheric $\boldsymbol{VCD_{trop}}$ fractions.

1. Calculating stratospheric ***BrO***. ***BrO*** $\boldsymbol{VCD_{strat}}$ is determined from a climatological approach, driven by SCIAMACHY $\boldsymbol{O_3}$ and $\boldsymbol{NO_2}$ observations. SCIAMACHY total $\boldsymbol{O_3}$ columns are used as a proxy for the stratospheric dynamics, while photochemical effects are taken into account using stratospheric $\boldsymbol{NO_2}$ columns (calculated using SCIAMACHY $\boldsymbol{NO_2}$ limb profiles).

2. Calculating strato- and tropospheric AMFs. Weighting functions (block AMFs) are read from a look–up table. They depend on five parameters including surface albedo and height, solar zenith angle and viewing geometry. For $\boldsymbol{AMF_{strat}}$ computation climatological ***BrO*** profiles are taken, whereas Gaussian profile with a maximum at 6 km hight is assumed in the troposphere.

Tropospheric *BrO* product (continued)

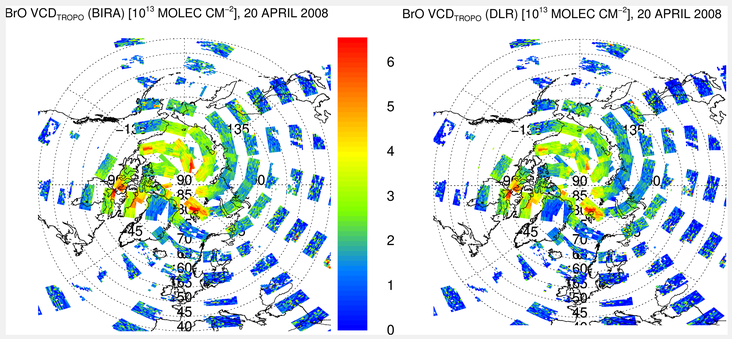
3. Subtracting stratospheric slant columns from total slant columns. The tropospheric slant column is computed as the difference between the nadir ***BrO*** total slant column and the stratospheric slant column: $\boldsymbol{SC_{trop} = SC_{total}^{nadir} - SC_{strat}}$.

4. Applying tropospheric AMF. Finally tropospheric ***VC*** is calculated as follows: $\boldsymbol{VC_{trop} = \frac{SC_{trop}}{AMF_{trop}}}$.

The algorithm needs total ***BrO*** and $\boldsymbol{O_3}$ columns together with stratospheric $\boldsymbol{NO_2}$ of the full orbit as input. Therefore it is implemented as a processing step that starts after the limb and nadir retrievals.

Tropospheric *BrO* product: verification results

- Verification data set: total of ∼200 orbits
- Reference data from scientific ***BrO*** product provided by BIRA.
- Polar maps of the SGP (prototype) and the reference algorithm results for 20th May 2008



- All bromine explosion events detected by both retrievals
- Planned for ESA's operational level 2 processor (version 7)

New L2 format

The Version 7 of the L2 SCIAMACHY data is to be released in a new more user-friendly and more suitable for the long-term data preservation NetCDF format. The SQWG aims to align and harmonize the new format with other missions (esp. Sentinels and GOME-1). Splitting of the L2 products into profile and column products is also considered. Additionally, reading routines for the new formats will be developed and provided.
The first version of the new format has been already created and the test file is made available for the members of the SQWG for further suggestions and revisions. The following guidelines have been pursued when designing the new format:
Completeness All information that was contained in the old level 2 files should also be contained in the new ones

Clean-up Elements of the old format that are no longer used, or may never be used, should not be ported to the new format

Clarity Elements of the old format that were difficult to understand, to access, to extract, or to handle, should be reorganized and represented in a more user-friendly way within the new file format

Compatibility, conformity and harmonization
- with data products of other instruments on ENVISAT, which have originally been delivered in the ENVISAT format, and for which a NetCDF-based format is considered
- with level 2 file formats of other instruments on past or future atmospheric chemistry missions, especially TROPOMI on Sentinel 5 Precursor
- with climate and forecast meta data conventions

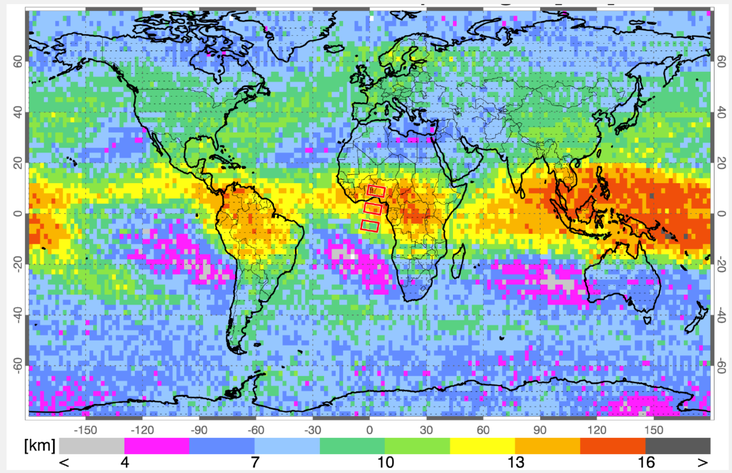
Cloud flagging using limb spectra

In limb mode SCIAMACHY measures light scattered along the line-of-sight. If the line-of-sight intersects a cloud at a certain height, the measurements differ from cloud free measurements. For the clouds detection, ratios of spectral measurements in two wavelength region are used (at 750 nm and 1090 nm). In an ideal atmosphere, consisting only of molecules, the difference between radiances at two wavelengths about 300 nm apart is large ($I \sim \lambda^{-4}$), while for larger particles like cloud droplets this difference is reduced ($I \sim \lambda^{-1}$).

The SCIAMACHY cloud detection algorithm (SCODA) [2] is already implemented in the L1b-2 operational processor (since version 5.02 released in 2012). SCODA considerably improved the limb trace gas retrievals in the upper troposphere/lower stratosphere region. Since then the scientific version of SCODA has been reviewed and further improved. These latest modifications are currently being implemented into the operational processor.

SCODA distinguished four different cloud types:
- water/ice/aerosol clouds (WCL)
- water/ice clouds (ICL)
- polar stratospheric clouds (PSC)
- noctilucent clouds (NLC).

Comparing to the previous version of SCODA small changes will be undertaken:
- geographical constraints for PSCs
- maximal solar zenith angle for which the detection is still performed
- maximal allowed and warning heights for all types of clouds
- updated thresholds for detection of all types of clouds



Global map (2°x2°) of the annual mean cloud top height (in km) for 2006. The superimposed red rectangles show the approximate size of three consecutive SCIAMACHY limb scans.

References

[1] N. Theys et al: Global observations of tropospheric BrO columns using GOME-2 satellite data. *Atmos. Chem. Phys.*, **11**, 1791–1811, 2011.

[2] K.-U. Eichmann et al: Global cloud top height retrieval using SCIAMACHY limb spectra: model studies and first results. *Atmos. Meas. Tech.*, **9**, 793–815, 2016.

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