BrO product specification document (version 1)

Chris Sioris
Harvard-Smithsonian Center for Astrophysics
csioris@cfa.harvard.edu February 19, 2006

Table of Contents

Product description

Each product file contains the BrO profile retrieved from a single limb scan. The observations are azimuthally averaged. The retrieved profile is given in number density (molec/cm^3). BrO is retrieved from 12 to 30 km, typically. There are approximately 9 retrieval levels, and vertical spacing between adjacent retrieval levels is 2 km. The actual vertical resolution is ~3 km. The number density reported at (*e. g.*) 15 km is effectively the number density in the 1 km thick layer between 15 and 16 km. The retrieval algorithm linear interpolates the number density between 15 and 17 km to obtain the number density at 16 km (*i.e.* in the 16-17 km interval) priori to each forward model iterations.

Data accompanying the retrieved BrO profile include the assumed air number density profile (in molec/cm^3) from the McLinden *et al.* [2002] database of model atmospheres, the assumed wavelength and month-dependent surface albedo (from GOME) at ~350 nm [Koelemeijer *et al.*, 2003], and the tangent height offset (in km), used to correct the tangent heights provided in the L1b product, based on the ~305 nm knee [Sioris *et al.*, 2003], but averaged over the entire orbit.

For more information on the algorithm, see the BrO algorithm document.

Product format specification

The data is currently stored in Microsoft Excel spreadsheet format (*.xls). Column C of each spreadsheet (rows 14-21) contain a list of input parameters and geographical information, including the tangent point azimuth difference and solar zenith angles, the reference tangent height (km), the surface albedo, the latitude of the retrieved profile, the latitude of the climatology, and the tangent height offset.
All input parameters are labeled in adjacent cells (column B).

The latitude of the retrieval is given by the average latitude of the tangent points for the elevation step at ~20 km (thus the latitude is azimuthally-averaged) and is located in cell C17. The product also contains the latitude selected from the latitude and month-dependent database of model atmospheres.
The retrieval altitude vector, the BrO number density profile and 1-sigma uncertainty are found in columns T,U and V (rows 12-22).

Software release history

This is the initial software release, namely version 1.

Implementation details

The following calibrations are applied to the L1b data using SciaL1C (EnviView 2.2.7):

- spectral
- pixel-to-pixel gain
- stray light
- etalon signature
- dark current

Selection criteria:
-the averaged SZA at 20 km is <90°
AND
-observed SCD uncertainty is <50% for at least one tangent height in the retrieval range

Analysis of observed spectra:
Fraunhofer reference: co-addition of limb spectra from same scan at tangent heights in ~33-70 km range.
Fitting window of observations: 344.1-360.0 nm

Absorption cross sections:
NO_2 - Bogumil *et al.* (2003) at 203, 223, 243 K
O_3: - Bogumil *et al.* (2003) at 203, 223, 243 K, corrected for solar I_0 effect
BrO - Wilmouth *et al.* (1999) at 228 K, corrected for solar I_0 effect

Closure polynomial: 3rd order

Temperature interpolation scheme in analyzing observed spectra: linear interpolation between SCDs from different temperatures to the temperature of the tangent altitude, using month and latitude-dependent temperature profiles from the McLinden *et al.* [2002] database.

Pseudo-absorbers:
1) 'tilt' [Sioris *et al.,* 2003]
2) de-trended ratio of the spectral radiance at the lowest reference tangent height to the co-addition of all of the other normalizing radiances

3) pseudo-absorber obtained by fitting the spectrum at the tangent height immediately below the lowest tangent height used in the retrieval with all the basis functions named above. The residual from this fit at a low tangent height is then used as a basis function in fitting all of the spectra at tangent heights included in the retrieval range.

Retrieval range: set to cloud top height, if cloud top > 12 km

Analysis of simulated spectra:

Fitting window of simulations: 344.10-359.85 nm
Wavelength step size, simulations: 0.21 nm

Reference TH, simulations: ~38 km

Absorption cross-sections:
NO_2 - Burrows *et al.,* 1998
O_3 - Burrows *et al.*, 1999
BrO - Wahner *et al.*, 1988

Closure polynomial: 3rd order

Convergence criteria: 3% (see Sioris *et al.* [2004] for more details)

List of known issues

Ideally, a high resolution O_3 cross section should be I_0-corrected rather than using a cross-section measured by the SCIAMACHY instrument. An I_0 correction to the SCIAMACHY cross-section is performed but this leads to some spectral smoothing because of the spectral resolution of SCIAMACHY is far from infinitesimal (~0.2 nm). The pointing correction applied in the current version of the data product is based on an outdated climatology of O_3 number density versus altitude. This can affect the pointing by ~1 km. The next version of the algorithm will update the O_3 climatology used to determine the pointing offset.
The L2 data does not include the filename of the L1b product used to generate it, the month, time, and geographical extent. All of this will be corrected in the next version of the data product.

Data quality assessment

The data agrees with DOAS balloon BrO to ~20%. The zonal repeatability is 2-3 pptv (parts per trillion by volume) and is fairly altitude-independent over the retrieval range. The improvements in this software release result from the solar I_0 correction of the BrO and O_3 cross sections. Also problems with the consistency of the definition of azimuth difference angle between observations and simulations no longer exist.

References

Aliwell, S. R., *et al.* (2002), Analysis of BrO in zenith-sky spectra: An intercomparison exercise for analysis improvement, *J. Geophys. Res.*, *107*(D14), 4199, doi:10.1029/2001JD000329.

Bogumil, K., *et al*. (2003), Measurements of molecular absorption spectra with the SCIAMACHY pre-flight model: instrument characterization and reference data for atmospheric remote-sensing in the 230–2380 nm region, *J. Photochem. Photobiol.*, *A 157,* 167–184.

Burrows, J. P., A. Richter, A. Dehn, B. Deters, S. Himmelmann, S. Voight, and J. Orphal (1999), *J. Quant. Spectrosc. Radiat. Transfer*, *61*, 509.

Burrows, J. P., A. Dehn, B. Deters, S. Himmelmann, A. Richter, S. Voight, and J. Orphal (1998), *J. Quant. Spectrosc. Radiat. Transfer*, *60*, 1025.

Koelemeijer, R. B. A., J. F. de Haan, and P. Stammes (2003), A database of spectral surface reflectivity in the range 335– 772 nm derived from 5.5 years of GOME observations, *J. Geophys. Res*., 108(D2), 4070, doi:10.1029/2002JD002429.

McLinden, C. A., J. C. McConnell, E. Griffioen, and C. T. McElroy (2002), A vector radiative transfer model for the Odin/OSIRIS project, *Can. J. Phys.*, *80*, 375-393.

Sioris, C. E., *et al.* (2003), Stratospheric profiles of nitrogen dioxide observed by Optical Spectrograph and Infrared Imager System on the Odin satellite, *J. Geophys. Res., 108*(D7), 4215, doi:10.1029/2002JD002672.

Sioris, C. E., T. P. Kurosu, R. V. Martin, and K. Chance (2004), Stratospheric and tropospheric NO_2 observed by SCIAMACHY: First results, *Adv. Space Res.*, *34*(4), 780-785.

Wahner, A., A.R. Ravishankara, S.P. Sander, and R.R. Friedl (1988), *Chem. Phys. Lett. 152*, 507.

Wilmouth, D. M., T. F. Hanisco, N. M. Donahue, and J. G. Anderson (1999), Fourier Transform Ultraviolet Spectroscopy of the $A^2\,\Pi_{3/2} \leftarrow X^2\,\Pi_{3/2}$ Transition of BrO, *J. Phys. Chem. A*, *103,* 8935-8945.