Algorithm Description

SCIAMACHY SO_2 Vertical Columns

Last changed: 02.03.2006

Data provider: Institute for Environmental Physics
University of Bremen
Otto-Hahn-Allee 1
D-28359 Bremen
Responsible Scientist: Andreas Richter
richter@iup.physik.uni-bremen.de
Internet: http://www.iup.physik.uni-bremen.de/doas

Forward Model:

The SO_2 Vertical Column product uses airmass factors derived with the radiative transfer model SCIATRAN (Rozanov et al., 1997), This model includes the effects of multiple scattering and atmospheric refraction and sphericity, but not polarisation.
The data analysis which is based on the DOAS technique (see next section) uses Lambert Beer's law of absorption and thus implies the "forward model" of an optically thin atmosphere.

Inversion Procedure:

The inversion procedure is based on the well known Differential Optical Absorption Spectroscopy (DOAS) method (e.g. Platt, 1994).

The basic concept of the DOAS retrieval on satellite measurements is application of Lambert Beer's law to the earthshine measurements using an absorption free direct solar irradiance measurement as background spectrum. To separate the effects of broad band extinction by Rayleigh and Mie scattering from the structured absorption by the trace species of interest, a polynomial of low order is fitted to the optical density simultaneously with the absorption cross-sections of all relevant absorbers. The resulting fit coefficient is the slant column density, i.e. the integrated amount of molecules per unit area averaged over all contributing light paths through the atmosphere.

Details on the implementation of the DOAS algorithm can be found in Richter, 1997; a description of the application to GOME data is given in Eisinger et al., 1998. Application to SCIAMACHY data has been reported in Afe et al., 2004.

The following settings have been used in the DOAS analysis:

Parameter	Value
wavelength window	315 - 327 nm
absorption cross-sections	SO_2 (Vandaele, 1994) O3 (Bogumil et al., 2003, 223 K & 243 K) Ring (Vountas et al., 1998) Undersampling
empirical functions used	Eta nadir Key data

degree of polynomial	cubic
offset and slope correction	offset and slope
background spectrum	ASM solar measurement from Dec. 15, 2002
normalisation	reference sector 180 - 230° longitude
data source	uncalibrated lv0 and lv1 data

Table 1: DOAS settings used for the SO_2 retrieval from SCIAMACHY measurements

For the vertical columns, a very simple airmass factor has been used which is based on a volcanic eruption profile with SO_2 situated between 10 and 15 km. This has implications on the data accuracy as discussed below.

Auxiliary Data:

No auxiliary data is used with the exception of the absorption cross-sections listed above and the vertical SO_2 profile used for the airmass factor calculation.

Sensitivity and Error Analysis and Algorithm Validation:

No dedicated algorithm validation has been performed. However, the same algorithm has been used for GOME SO_2 column analysis (Eisinger et al. 1998). Comparison of the GOME and SCIAMACHY data products shows good agreement. Some differences remain which are related to the improved spatial resolution of SCIAMACHY and the difference in time of measurements.

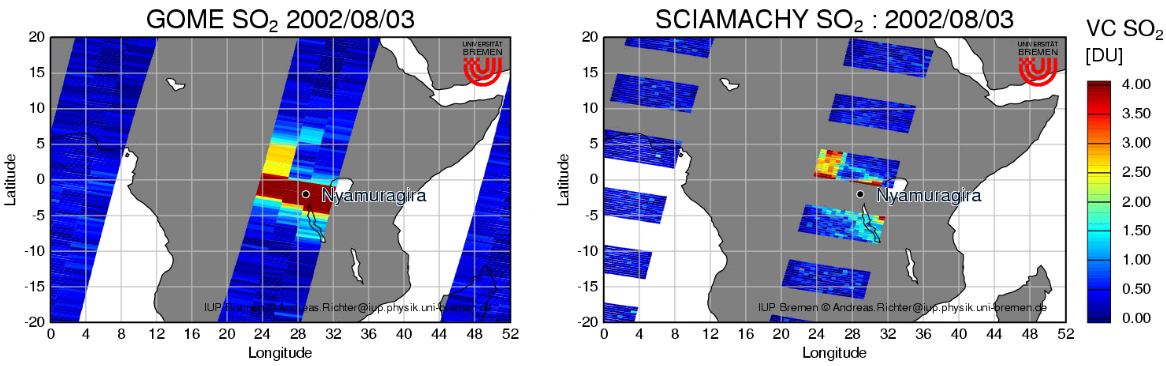

Fig. 1: Comparison of GOME (left) and SCIAMACHY SO_2 vertical columns for an overpass over the Nyamuragira volcano on August 3, 2002. SCIAMACHY measurements have better spatial resolution but less coverage owing to the alternating limb nadir measurements. The time difference between the two measurements is about 30 minutes.

Compared to GOME measurements, the SCIAMACHY SO_2 columns have larger scatter, mainly as result of the reduced ground pixel size.

The SO_2 retrieval has several problems which impact on the data quality:

- at large ozone absorption (large solar zenith angle, large ozone column), a spectral interference leads to unrealistic SO_2 columns
- there is a systematic difference between measurements over low and high terrain of unexplained origin which leads to lower values over elevated areas
- an offset which also varies with latitude and time is present in the data. The magnitude of this offset depends on the fitting window chosen.

To correct for this offset, the SO_2 columns over a reference sector (180 - 230° longitude) is subtracted from the measurements. While this compensates most of the effect and also some of the ozone interference, but still some problems remain even in the corrected fields. In cases where a volcanic SO_2 plume is present in the reference sector, the values elsewhere are too low at the corresponding latitude band.

The use of a simplified airmass factor has a large impact on the data product:

- over dark surfaces, the SO_2 is underestimated, in particular if it resides close to the surface e.g. in polluted areas
- over bright surfaces, SO_2 in the middle and upper troposphere is overestimated which leads to enhanced columns over snow and ice and also over low clouds.
- generally the airmass factor depends critically on altitude, and for a quantitative product, a dedicated airmass factor has to be computed for each volcanic plume or pollution scenario.
- for very large SO_2 concentrations, saturation effects occur and the airmassfactor also depends on the SO_2 vertical column.

No cloud clearing has been applied to the SO_2 product. Thus, in some measurements SO_2 might be hidden below a cloud while in others SO_2 in the free troposphere might be overestimated.

Recommendations for Product Validation:

Validation of SO_2 vertical columns should concentrate on situations with high signal such as volcanic eruptions or strong boundary layer pollution. For the latter, different airmass factors have to be computed and a more appropriate SO_2 product is available on request from Andreas.Richter@iup.physik.uni-bremen.de.

As for all tropospheric observations, the large footprint of SCIAMACHY measurements has to be taken into account for SO_2 validation.

References:

Afe, O. T., A. Richter, B. Sierk, F. Wittrock and J. P. Burrows, BrO Emission from Volcanoes - a Survey using GOME and SCIAMACHY Measurements, *Geophys. Res.Lett.*, **31**, L24113, doi:10.1029/2004GL020994, 2004

Bogumil, K., Orphal, J., Homann, T. Voigt, S., Spietz, P., Fleischmann, O. C., Vogel, A., Hartmann, M., Bovensmann, H., Frerik, J., and J.P. Burrows, 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, 2003

Eisinger, M., and J. P. Burrows (1998), Tropospheric sulfur dioxide observed by the ERS-2 GOME instrument, *Geophys. Res. Lett.,* 25, 4177– 4180.

Platt, U., Differential optical absorption spectroscopy (DOAS), 1994: in Air Monitoring by Spectroscopic Techniques, Chem. Anal. Ser., vol. 127, edited by M. W. Sigrist, pp. 27–84, John Wiley, New York

Richter, A., Measurements of stratospheric trace species above Bremen, 53°N using absorption spectroscopy, PhD thesis, University of Bremen, 1997 (in German)

Rozanov, V., Diebel, D., Spurr, R. J. D. & Burrows, J. P., GOMETRAN: A radiative transfer model for the satellite project GOME - the plane parallel version, *J. Geophys. Res.*, **102**, 16683-16695, (1997).

Vandaele, A. C., P. C. Simon, J. M. Guilmot, M. Carleer, R. Colin, SO2 absorption cross section measurement in the UV using a Fourier transform spectrometer, *J. Geophys. Res.,* **99**(D12), 25599-25606, 10.1029/94JD02187, 1994.

Vountas, M., V. V. Rozanov, and J. P. Burrows, Ring effect: Impact of rotational Raman scattering on radiative transfer in earth's atmosphere, *J. Quant. Spectrosc. Radiat. Transfer*, **60**, 943–961, 1998.