Product Specification Document: O_3, version >= 2.0

(Retrieval of O_3 vertical profiles from SCIAMACHY limb measurements at the University of Bremen, processing version >= 2.0)

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1 Product Description

The product contains vertical profiles of ozone retrieved from SCIAMACHY limb measurements at the University of Bremen. The results are given as number densities in $molecule/cm^3$ and as volume mixing ratios in ppV at 1 km altitude grid between 10 to 80 km. Please note, that the number densities are the primary retrieval product whereas volume mixing ratios are calculated from the retrieved number densities using the pressure and temperature from the ECMWF database. Here, the reanalysis ECMWF model with a spatial resolution of $5° \times 5°$ and a temporal resolution of 6 hours is used. Retrievals are done for azimuthally averaged measurements, i.e., only one profile per limb measurement sequence (also referenced as limb state) is retrieved. Additionally, the product contains a priori ozone profiles used in the retrieval as well as error estimations in both number density and volume mixing ratio representations. The vertical resolution of the retrieved profiles is about 3 km. The retrieval is based on the Level 1 data version 6.03. A detailed description of the retrieval process is given in the Algorithm Document available at `http://www.iup.physik.uni-bremen.de/~sciaproc/CDI/DOCU/Algorithm_Document.pdf`

2 Data Format

The vertical profiles of ozone retrieved from SCIAMACHY limb measurements and corresponding averaging kernels are stored in individual files in ASCII format, i.e., two files per limb measurement at each azimuth angle are generated. The names of the data files contain the date, the orbit number, the sequential number of the limb state in the orbit starting from "`00`", the number specifying the total number of retrieved azimuthal measurements per limb state (always "`1`" for this retrieval), the sequential number of the measurement in the azimuthal scan starting form "`0`"(always "`0`" for this retrieval), as well as the version of the retrieval algorithm. The profile files have an extension "`dat`" whereas the extension of the averaging kernel files is "`ak`". For example, `20050103_Orb14878_St07_Az1_0_V2_2.dat` and `20050103_Orb14878_St07_Az1_0_V2_2.ak` are the names of the files containing ozone vertical profiles and corresponding averaging kernels, respectively.

The format of the output files containing the vertical profiles of atmospheric species (data files having the "`dat`" extension) is as follows:

```
# Product            :  O3 vertical profiles from limb measurements
# Scientific contact :  Dr. Alexei Rozanov (Alexei.Rozanov@iup.physik.uni-bremen.de)
# Retrieval version  :  V2.2
# Cloud detection    :  SCODA V1.3
# Data source        :  SCI_NL__1PRDPA20050103_105552_000060312033_00295_14878_8978
# Orbit nr.,State ID :  14878 29
# Ver. Proc/Key/M/I/D:  SciaL1c/6        03.10 -1.
# Applicator version :  Version 6 $Revision:  1.24 $
# Calibr. appl. (0-8):  0 1 2 3 4 5
# State Starttime    :  03-Jan-2005 11:23:28.179664
# Nr Profiles / act. :  1 0
# Satellite height   :  796.32
# Earth radius       :  6396.72
# Solar zenith angle @TP : 77.11
# Average Lat & Long @TP : 51.79 348.15
# Ground pixel latitudes :  53.52 51.50 50.40 52.08
# Ground pixel longitudes:  342.16 354.07 353.65 342.64
# Total column, DU        :  223.204317082248
# Altitude [km], concentration [mol/cm3], error [mol/cm3], a priori [mol/cm3], volume mixing ratio,
# VMR error, VMR a priori, cloud flag, cloud type, PSC flag
80.00 0.1645E+08 0.1641E+06 0.1645E+08 0.5874E-07 0.5860E-09 0.5874E-07 0 -1 -1
79.00 0.2158E+08 0.2152E+06 0.2158E+08 0.6768E-07 0.6751E-09 0.6768E-07 0 -1 -1
78.00 0.2795E+08 0.2787E+06 0.2795E+08 0.7697E-07 0.7677E-09 0.7697E-07 0 -1 -1
.....
12.00 0.9540E+12 0.1867E+12 0.2846E+13 0.1387E-06 0.2713E-07 0.4137E-06 2 -1 -1
11.00 0.6079E+12 0.1388E+12 0.2508E+13 0.7771E-07 0.1775E-07 0.3206E-06 2 -1 -1
10.00 0.2502E+12 0.5941E+11 0.2058E+13 0.2840E-07 0.6743E-08 0.2336E-06 2 -1 -1
```

The product name in the first header line of each data file gives a basic description of the file contents, i.e., retrieved atmospheric species, type of the contained information (e.g., vertical profiles), and type of SCIAMACHY measurements which this information was inferred from. The second header line contains the name and the e-mail address of the scientific contact person. The version number of the processing chain contained in the third header line allows users to trace back the version numbers of the software involved in the retrieval process as well as retrieval parameter settings. The version numbers for different species are independent, i.e., the same version number for different atmospheric species does not mean that the same software and parameter settings were used. The fourth header line contains the name and the version number of the cloud detection algorithm used to set cloud flags in data columns 8 – 10 (see below). The fifth header line contains the name of the Level 1 data file used for the retrieval and the sixth header line contains orbit number and state ID of the corresponding measurement. Three subsequent header lines contain the version number of the Level 1 data file, information on the applicator software used to extract Level 1c dataset, and the calibration flags used by the applicator software. Next header line contains the date and time information relevant for the unique identification of the measurement. The eleventh header line provides information on the azimuthal averaging, i.e., how many azimuthal measurements per limb state are retrieved. The second value in this header line specifies the sequential number of the current measurement in the azimuthal scan starting from zero. Next two header lines contain information on the satellite altitude and local Earth radius. The four subsequent header lines contain the solar zenith angle at the tangent point (averaged over the measurement) as well as average geolocation of the limb measurement and ground pixel coordinates. The last header line contains the ozone total column in Dobson units obtained integrating the number density profile from the bottom to the top of the atmosphere

(usually 0 and 100 km, respectively). In altitude regions where the retrieval sensitivity is poor, a priori information is used in the integration procedure. The header lines are followed by the data block comprising the altitude information in km (first column), profile information (second to seven columns) and cloud flags (eighth to tenth columns). The profile information block contains the retrieved vertical distribution of the number density, corresponding retrieval error, a priori profile in molecules/cm^3, volume mixing ratios corresponding to the retrieved number densities, appropriate retrieval errors, as well as a priori profile in the volume mixing ratio representation. The cloud flags specified in eighth to tenth columns are set for each altitude independently. The first column in the cloud flagging block contains general cloud flag specifying if any cloud is detected at the corresponding altitude. The following values can appear here: "0" - no cloud detected, "1" - thin cloud or partially clouded scene, "2" - thick widely extended cloud. The cloud flag in the second column of the cloud flagging block describes the type of the selected cloud, namely, "0" means a water cloud and "1" means an ice cloud. The cloud flag in the third column of the cloud flagging block indicates if a polar stratospheric cloud (PSC) was detected ("0" or "1"). If the required information was not found in the cloud data base, the value "-1" will appear. In this case, the remaining information is not affected and can still be used.

The averaging kernels corresponding to the retrieved vertical profiles of ozone are stored in the files having the same names as the profile files and the extension "`ak`" instead of "`dat`". No header is supplied for the averaging kernels, instead, the geolocation and other auxiliary information can be obtained from the header of the corresponding profile file. The first line of each averaging kernel file contains the altitude grid at which the averaging kernels are written out. The altitude grid is the same for both dimensions of the averaging kernel matrix. Typically, the altitude grid remains the same for all retrievals of the same processing version, however, it does not need to match the altitude grid of the retrieved vertical profiles. Separated by a blank line, the averaging kernel matrix is written out with the first dimension running with the row number, i, (vertically) and the second dimension running with the column number, j, (horizontally) in accordance with the following definition:

$$\mathbf{x}_i = \mathbf{x}_i^a + \mathbf{x}_i^a \sum_j \mathbf{A}_{i,j} \frac{\mathbf{x}_j^t - \mathbf{x}_j^a}{\mathbf{x}_j^a} ,$$

where i and j denote the elements of the vectors or matrices, and $\mathbf{x}$, $\mathbf{x}^a$, and $\mathbf{x}^t$ are the retrieved, a priori, and true profiles respectively.

The entire dataset is distributed between several subdirectories according to the target species names which contain yearly, monthly, and daily grouped retrieval results. Thus, for example, vertical distributions of ozone retrieved from SCIAMACHY limb measurements performed on March 10^{th}, 2003, are located in `O3/2003/03/10` subdirectory. The profiles and averaging kernels are tared/gziped orbitally. To make the data transfer more easy, individual limb states are additionally stored in daily tar-archives which are located in `tar` subdirectory of the corresponding `Gas/Year/Month` directory. For example, the `O3/2003/03/tar` directory contains daily tar-files for March 2003.

3 Implementation Details and Software Release History

3.1 Current version: 2.2

- Forward model: SCIATRAN 3.0
- Spectral region: 2 nm spectral intervals centered around: 264 nm, 267.5, 273, 283, 286, 288, 290.5, and 305 (UV) as well as 525, 589, and 675 nm (Chappuis band)
- Surface albedo: geographical database [Matthews, 1983]

- Clouds treatment: neglected in the retrieval, cloud information included in the output files
- Aerosol parameterization: LOWTRAN background aerosols [Kneizys, 1996]
- Weighting functions type: single scattering
- Atmospheric species in the forward model: O_3
- Retrieved Atmospheric species: O_3
- Reference tangent height number: 24 ($\approx$ 72 km), 24, 24, 23 ($\approx$ 69 km), 22 ($\approx$ 66 km), 22, 21 ($\approx$ 62 km), and 19 ($\approx$ 56 km) for UV wavelengths, respectively, as well as 15 ($\approx$ 43 km) for the Chappuis triplet
- Tangent heights selected for the retrieval: 18 – 24 ($\approx$ 53 – 69 km), 18 – 24, 18 – 24, 16 – 22 ($\approx$ 46 – 66 km), 16 – 22 ($\approx$ 46 – 62 km), 16 – 22, 16 – 21 ($\approx$ 46 – 59 km), and 13 – 19 ($\approx$ 37 – 53 km) for UV wavelengths, respectively, as well as 5 – 14 ($\approx$ 10 – 40 km) for the Chappuis triplet
- Spectral smoothing: averaging over 2 nm intervals
- A priori uncertainty: 1000%
- Signal to Noise Ratio: 15, 15, 15, 30, 30, 30, 30, and 50 for UV wavelengths, respectively, as well as 140 for the Chappuis triplet
- Correlation length: 1.5 km
- Additional regularization: Tikhonov smoothing (smoothing parameter linearly decreases with altitude from 9 at 72 km to 3 at 7 km)
- Solution method: Optimal estimation type
- Iterative scheme: Newton

3.2 Changes in version 2.2 with respect to the previous version (2.1)

- Foward model is changed from SCIATRAN 2.2 to SCIATRAN 3.0 (this is done due to technical reasons only, the retrieval results are identical for both SCIATRAN versions)
- Surface albedo database is used instead of a constant value of 0.3

3.3 Changes in version 2.1 with respect to the previous version (2.0)

- The central wavelenght of the Chapuis triplet is shifted from 601 to 589 nm
- Tikhonov parameter linearly decreases with altitude from 9 at 72 km to 3 at 7 km instead of constant value of 6

References

E. Matthews, Global vegetation and land use: new high-resolution data bases for climate studies, *J. Clim. Appl. Meteor.*, 22, 474-487, 1983.

Kneizys, F., L. Abreu, G. Anderson, J. Chetwynd, E. Shettle, A. Berk, L. Bernstein, D. Robertson, P. Acharya, L. Rothman, J. Selby, W. Gallery, and S. Clough, The MODTRAN 2/3 report and LOWTRAN 7 model, Tech. Rep., contract F19628-91-C-0132 with Ontar Corp., Phillips Laboratory, Hanscom AFB, 1996.