Belgian Institute
for Space Aeronomy

BIRA-IASB

Sulphur Dioxide Data Service

Product Specification Document

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1 Introduction

1.1 Purpose of this document

A Sulphur Dioxide Data Service has been set up by BIRA-IASB, in collaboration with KNMI and DLR, in the framework of the projects TEMIS, PROMOTE and SACS. This Service has two branches:

- Archive Service
- NRT Service

The data are accessible via the TEMIS and SACS websites: http://www.temis.nl/aviation/so2.php and http://sacs.aeronomie.be/

This document describes the specifications of the data products of the Sulphur Dioxide Data Service. The latest version of this document can be found on the SO2 Products Info Service website at http://sacs.aeronomie.be/info/docs.php

The Data and Service version history is given in section 2.1 of the *Product Specification Document* [PSD].

1.2 Acronyms and abbreviations

AMF	Air-Mass Factor
BIRA-IASB	Belgian Institute for Space Aeronomy
DLR	German Centre for Air and Space Research
DOAS	Differential Optical Absorption Spectroscopy
DU	Dobson Units
ESA	European Space Agency
HDF	Hierarchical Data Format
KNMI	Royal Netherlands Meteorological Institute
NOVAC	Network for Observation of Volcanic and Atmospheric Change
NRT	Near-real-time
PROMOTE	Protocol Monitoring for the GMES Service Element: Atmosphere
SCD	Slant Column Density
SO2	Sulphur Dioxide
SZA	Solar Zenith Angle
TEMIS	Trophospheric Emission Monitoring Internet Service
VCD	Vertical Column Density

1.3 Applicable documents

[ADD] Algorithm Description Document: BIRA_SO2_ADD_v11r1.doc
[PSD] Product Specification Document: BIRA_SO2_PSD_v11r1.doc

1.4 Credits

The SO2 Data Service is set up and distributed as part of the following projects:

TEMIS -- Tropospheric Emission Monitoring Internet Service
http://www.temis.nl/

PROMOTE -- Protocol Monitoring for the GMES Service Element
http://www.gse-promote.org/

SACS -- Support to Aviation Control Service
http://sacs.aeronomie.be/

by the Belgian Institute for Space Aeronomy (BIRA-IASB, Brussels, Belgium) in collaboration with DLR (Oberpfaffenhofen, Germany) and KNMI (De Bilt, The Netherlands).

BIRA-IASB
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2 General product description

Sulphur dioxide (SO2) slant column densities in Dobson Units (DU) are retrieved for each ground pixel of the nadir observations of SCIAMACHY. The data delivery is limited to observations at solar zenith angles less than or equal to 85 degrees. Along side the slant column density (SCD) the retrieval error on the SCD (in DU) and the chi-square of the fit are given.

A correction for the average background SO2 level and for the interference between the absorption signals of SO2 and ozone at high solar zenith angle is applied to the SCD.

A vertical column density (VCD) is also part of the data product.

For a description of the slant column retrieval method (DOAS technique) and the background correction, see the *Algorithm Document* [ADD].

The SO2 Data Service has two branches:

- Archive Service
- NRT Service

The Service provides global data files and maps (daily and monthly average maps). Higher resolution maps over pre-defined regions known for SO2 emission from volcanic activity (41 regions of 30 by 30 degrees) are provided as well.

2.1 Data and Service version history

The data files, and with that the Services, have been given a version number, in order to track changes in the different parts of the processing.

The version number looks like this: `A.B.C`

where `A.B` represents the version of the slant column retrieval and the warning system, and `.C` the version of the AMF-based vertical columns; if `C` is zero or absent, no vertical columns are available. Note that the combination `A.B` is used as version number of the documentation.

The table below gives an overview of the version numbers and what was added/done for that version. Additions to the website of the data record, which do not merit an increase of the version number, are not mentioned here.

Version	***Date***	***Description***
1.0.3	July 2010	Plot of imaging has been re-processed for all the NRT and archive service. A solar zenith limit angle is now considered with a seasonal dependency to avoid problem of measurements for the North and South Pole. A plume height of about 15 km is also considered for SCIAMACHY and GOME-2 to decrease the noise of instruments. An update of archive in real-time (with GOME-2 and SCIAMACHY data) takes place now. Update of archive system (July 2010).
1.0.3	October 2009	Alert system in function considering only SCIAMACHY data. Update of archive system (October 2009).
1.0.3	February 2008	Near-real time images of GOME-2 based SO2 data are made available, using a preliminary background correction (compensating mainly for an offset). Once more experience is gained with GOME-2 data, the background correction will be improved, and the data will also be made available.
1.0.3	January 2008	The colour scale of the SO2 vertical column plots in the archive has been adapted: it now ends at 2 DU (was 3), so that large SO2 values are better visible (the SO2 slant column values are usually larger and their colour scale ends at 3 DU). The colour scale of the NRT processing is adapted on 07 Jan.
1.0.3	November 2007	Near-real time images of OMI SO2 data are made available; the NRT data itself is not available for third parties. An archive of the OMI data will follow later.
1.0.3	August 2007	Introduction of a new, improved background correction in the processing, in particular to try to get rid of most of the of artifacts at high SZA, giving rise to "false alerts" due to the interference between the absorption signals of SO2 and ozone. At the same time VCDs are included in the processing, the data format of the files has been adapted and the presentation on the web site has been improved. A separate page gives a full overview of the new faetures of version 1.0.3. Initially, the archive covers the months January to June 2007; more data is added later. The near-real time processing and alert service were started on 16 August; the preceeding days of that month were processed by hand as if in NRT.
0.9	February 2007	Automatic notification by e-mail of "exceptional SO2 concentrations" made public. The details of this service have not yet been incorporated in the on-line product information. Due to the interference between the absorption signals of SO2 and ozone, there are quite a lot of artifacts at high SZA, giving rise to "false alerts". An

		improved background correction, to get rid if these artifacts, is under investigation.
0.9	November 2006	Added a new Volcano region, to cover three remaining volcanoes with a last known eruption after 1800 in Turkey and Syria. This new region has number 5, and inserting it required renumbering most regions. Where necessary data files and images have been updated accordingly. There are now 42 volcano and 11 air quality regions. Update of the on-line product information, and offering the possibility to download that as one printable document in the Documents section.
0.9	September 2006	Start of the Near-real time processing service, providing data and images to the website; the notification of exceptional SO2 concentrations is not available yet.
0.9	June 2006	Complete re-analysis and re-plotting of all data on the website (Sept. 2004 - Jan. 2006) because of an improved background correction for the SO2 slant column. At the same time, the FRESCO cloud cover fraction is included in the data product and as images on the website, to assist interpreting the results All data files (ASCII and HDF) and all images are therefore renewed. The product information web pages and the pages presenting the data have been adapted accordingly. *Note that these improvements have changed the format of both the ASCII and the HDF data files.* The documents that can be downloaded from the Downloadable documentation page are *not* yet updated to version 0.9. *Later data additions for this version:* • Slant column data and images for 2006: February, March, April • Colour scale of cloud fraction plots improved.
0.8	November 2005	Improved data file header (in preparation for addition of VCD data) and a correction of the "relative azimuth angle" (error in previous version). This applies to the ASCII data files only; the HDF data files remain version 0.7.
0.7	October 2005	Full SO2 Archive Services set up, with an improved background correction,improved web access to the different archives, and a more extensive product information

0.6	December 2004	Prototype SO2 Archive Service set up, with preliminary on-line product information
--	Up to mid 2004	Preliminary data processing from GOME and SCIAMACHY for 2000 to mid 2004, without any correction for the background SO2 levels; these data sets and images will be replaced by new processing.

Some more details on the changes and additions per version number can be found in the on-line product information under “Data and Service version history” at http://sacs.aeronomie.be/info/version.php

Note:
Version 0.8 was the first version to be documented on paper; some product information was available via the website as of version 0.6.

3 Data product format specification

Slant column data is delivered in two major forms:

- ASCII data at the coordinates of the SCIAMACHY observations, one entry per ground pixel, one level-2 file per level-1 file – this data product is generated for the Archive Service.

- HDF data at a rectangular latitude-longitude grid for daily data (i.e. all orbit starting at one date put together), and monthly averages – this data product is generated for the Archive Service.

The data product files mention, among others, version number (see section 2.1) and the files have been given a *product status*.

The data products are available at:
http://sacs.aeronomie.be/archive/index.php?InstruSCIA=1&obsVCD=1&modeONE=1

3.1 ASCII data file specification

ASCII data files provide data at the coordinates of the SCIAMACHY observations, one entry per ground pixel, one level-2 file per level-1 file.

3.1.1 Data file name

For a given day, the orbits treated are those orbits that have a start time during that day; this is the time mentioned in the name of the data file. The name of the SO2 data files contains the orbit date `YYYYMMDD` and the orbit start time `HHMMSS`, both taken from the original measurement file:

`sciaYYYYMMDD_HHMMSS.dat`

`gome2YYYYMMDD_HHMMSS.dat`

where `scia and gome2` stands for SCIAMACHY and GOME-2 instruments. These files contain the SO2 slant column data (SCD) with no background correction and the SO2 vertical column density (VCD) derived with an appropriate air-mass-factor (3 types of AMF available according to 3 estimations of plume height at 2.5 km, 6.5 km and 14 km).

3.1.2 Data file format

Each data file has a header with comment lines (starting with the # mark), giving information on the data columns. A typical data file header for data files containing only SCD data looks as follows. Some remarks regarding the entries in the file header are given further down.

```
# SO2 column density for TEMIS / PROMOTE
# ---------------------------------------
#
# Product status  : preliminary data
# Process version : 0.8
#
# Instrument      : SCIAMACHY
# Orbit date/time : 20050501_125219
# Orbit number    : 16568
#
# Analysis date   : 2005/11/17
#
# Data columns                                          [format]
#
# --- Ground pixel data
#     1 = measurement date as YYYYMMDD                  [a8]
#     2 = measurement time as HHMMSS.SSS                [1x,a10]
#     3 = pixel id: 0=foreward, 3=backsan               [i4]
#   4-7 = pixel corner latitudes                        [4f9.3]
#     8 = pixel center latitude                         [f9.3]
#  9-12 = pixel corner longitudes                       [4f9.3]
#    13 = pixel center longitude                        [f9.3]
#    14 = solar    zenith  angle (SZA) at TOA           [f9.3]
#    15 = viewing  zenith  angle (VZA) at TOA           [f9.3]
#    16 = relative azimuth angle (RAA) at TOA           [f9.3]
#
# --- Slant column data
#    17 = SO2 slant column density SCD  (in DU)         [f9.3]
#         with background corr. for daily plots
#    18 = SO2 slant column density SCD  (in DU)         [f9.3]
#         with background corr. for monthly averages
#    19 = retrieval error on the SCD    (in DU)         [f9.3]
#    20 = chi^2 of the slant column fit (x 1e-6)        [f9.3]
#    21 = slant column value index (SVI)                [i4]
#         0 : SO2 SCD <= 1.5 DU
#         1 : SO2 SCD >  1.5 DU, no warning issued
#         2 : SO2 SCD >  1.5 DU, warning issued for state
#
# 22-23 = SCIAMACY state_index and state_id             [2i4]
#
#
# Full data format: (a8,1x,a10,i4,17f9.3,3i4)
#
#
```

Which is followed by two lines spanning all the columns and giving a header to each column. Then follow the data lines themselves. The very end of the file is marked by:

```
#
# --- end of file.
```

Remarks regarding some of the entries in the above file header:

- On the right of the list of data columns and below the list is the format with which the data can be read in the notation used, for example, in Fortran and IDL.
- Column 3 gives the type of ground pixel. For SCIAMACHY data there is only a distinction between forward and backward scan pixels. For GOME data the forward pixels pixels come in three types, for which the number 0, 1 and 2 will be used.
- The zenith and azimuth angles (columns 14, 15 and 16) are given at the top-of-atmosphere (TOA) for the centre of the ground pixel.
- The SO2 slant column value in column 17 is used for making the plots of the daily data and the 3-day composites, the value in column 18 for monthly (and higher) averages. The difference between the two is due to the use of a different background correction. *NOTE: this distinction will be removed in a future release and only one type of SCD will be given.*
- The error value given in column 19 is the error following from the DOAS slant column retrieval. Its value is based on the RMS of the fit between the measured and the fitted spectrum. The chi-square in column 20 is also a measure of the quality of the fit. In fact, these three quantities are all interlinked: chi-square = RMS * RMS, and the relationship between the slant column error and the RMS is assumed to be linear. To assist the data user in her/his analysis, both the slant column error and the chi-square are written to the data file.
- The "slant column value index" (SVI) in column 21 is meant to give the user a quick look facility on the SO2 slant column value. For more information, see the chapter on the criteria for SO2 warnings.

3.2 HDF data file specification

HDF data files provide at a rectangular latitude-longitude grid for daily data (i.e. all orbit starting at one date put together), three-day composites, and monthly averages.

For the moment the spacing of the latitude-longitude grid is 0.5 by 0.5 degrees; in a future version this will be reduced to 0.25 by 0.25 degrees.

3.2.1 Data file name

The name of the HDF file depends on the data period covered by the file and is constructed as follows:

`sciaYYYYMMDD.hdf`	File with data for a single day; the name contains the orbit date YYYYMMDD
`so2cdYYYYMM.hdf`	File with data for a monthly average; the name contains the year and month

3.2.2 Data file format

An HDF file with just the SO2 slant column data has the following structure:

- File header, with the file attributes specifying the product name, data, version, units, etc.
- Data sets:
  1. SO2 slant column field
  2. Error in the slant column field (from the slant column retrieval)

If the SO2 vertical column is available, the file will have more data sets.

The following table gives as an example the header of the HDF file of the daily slant column data of 10 December 2004.

Global Attribute	***Type***	***Value***
Product	string	SO2 slant column [DU]
Data_version	string	0.7
Creation_date	string	7 October 2005
Product_status	string	preliminary
SO2_field_date_1	integer	2004, 12, 10
SO2_field_date_2	integer	2004, 12, 10
Data_begin	integer	2004, 12, 10, 2, 19, 54
Data_end	integer	2004, 12, 11, 0, 54, 56
Date_format	string	year, month, day, hour, minute, second (UTC)
Instrument	string	SCIAMACHY (ENVISAT)
Authors	string	Jos van Geffen & Michel Van Roozendael
Affiliation	string	BIRA-IASB (Belgian Institute for Space Aeronomy)
E-mail	string	Jos.VanGeffen@bira-iasb.be & Michel.VanRoozendael@bira-iasb.be

Number_of_longitudes	integer	720
Longitude_range	real	-179.75, 179.75
Longitude_step	real	0.50
Number_of_latitudes	integer	360
Latitude_range	real	-89.75, 89.75
Latitude_step	real	0.50
Iscd_field	string	SO2 slant column field
Iscd_error	string	Error on SO2 slant column field
Field_unit	string	Column = Iscd_field/1000 [DU]
Error_unit	string	Error = Iscd_error/1000 [DU]
No_data	string	Entries with -99.0 DU represent "no data"
Product_code	string	ssndap
Data set	***Type***	***Rank --> dimensions***
Iscd_field	integer	2 --> 720 x 360
Iscd_error	integer	2 --> 720 x 360

Remarks regarding some of the attributes in the file header:

Product
This attribute gives so to say the title of the product. In the example it says that the file has SO2 slant column data for one day.

- For 3-day composites " – 3-day composite" is added.
- For monthly averages " – monthly average" is added.
- ... etc.

If the file contains slant column as well as vertical column densities, the main title is "SO2 column densities [DU]".

SO2_field_date_#
These two attributes give the period for which the data applies in whole days (UTC). In the example above this is one day; for longer time periods they give the first and last day.

Data_begin & Data_end
These two give the date and time of the very first and the very last measurement included in making the gridded data.
Measurements of SCIAMACHY and GOME-2 come in principle in files at one file per orbit. The data included is from al data files which have a start time in the given period. The last orbit of a given day can, of course, continue into the next day. In that case "Data_end" shows the beginning of the next day, as in the above example. See also section 4.6 on this.

Longitude & latitude ranges and steps
These are given in degrees, with negative values for West longitudes.

Data sets

The above example is for a file which contains only the slant column density, with 'scd' in the name of the data set. Files with also vertical column densities have more data sets, with 'vcd' in the name of the data set (e.g. "vcd_field").

Product code
This is for internal use, to ease post-processing.

4 Further product information

4.1 Known issues

This section describes some issues to keep in mind when using the data products, in addition to the remarks made in Chapter 4.

4.1.1 South Atlantic Anomaly

The Van Allen radiation belts are doughnut-shaped regions of high-energy charged particles trapped by the Earth's magnetic field. The inner radiation belt, discovered by James Van Allen in 1958 with the Explorer 1 and 3 missions of NASA, occupies a relatively compact region above the equator roughly between 40 degrees north and south.

The Earth's magnetic dipole field is offset from its centre by about 500 km. As a result of this, the inner Van Allen belt is on one side closer to the Earth's surface. This region is named the South Atlantic Anomaly (SAA) and it covers a part of South America and the southern Atlantic Ocean: it lies roughly between latitudes 5 and 40 degrees South, and between longitudes 0 and 80 degrees West – the precise strength, shape and size of the SAA varies with the seasons.

This dip in the Earth's magnetic field allows charged particles and cosmic rays to reach lower into the atmosphere. Low-orbiting satellites, such as ERS-2 and ENVISAT, pass daily through the inner radiation belt in the SAA-region. Upon passing the inner belt, charged particles may impact on the GOME detector, causing higher-than-normal radiance values. The impact of charged particles on the GOME and SCIAMACHY detectors decreases the quality of the measurements, i.e. the signal-to-noise ration, of earthshine spectra, notably in the UV.

This reduction of the signal-to-noise also affects the retrieval of SO2 slant columns: in the SAA region the variation in slant column values is much higher than elsewhere. This shows up clearly, for example, in the monthly average, as the image below illustrates. The decreased signal-to-noise may result in artifacts in the SO2 slant columns. For this reason, neither the Volcanic SO2 nor the Air Quality SO2 Service has a geographic region defined in the area of the South Atlantic Anomaly.

Figure 6 shows, as an example, the monthly average SO2 slant column for January 2005. Note the increased noise in the SO2 slant column over South America, which can be attributed to the South Atlantic Anomaly.

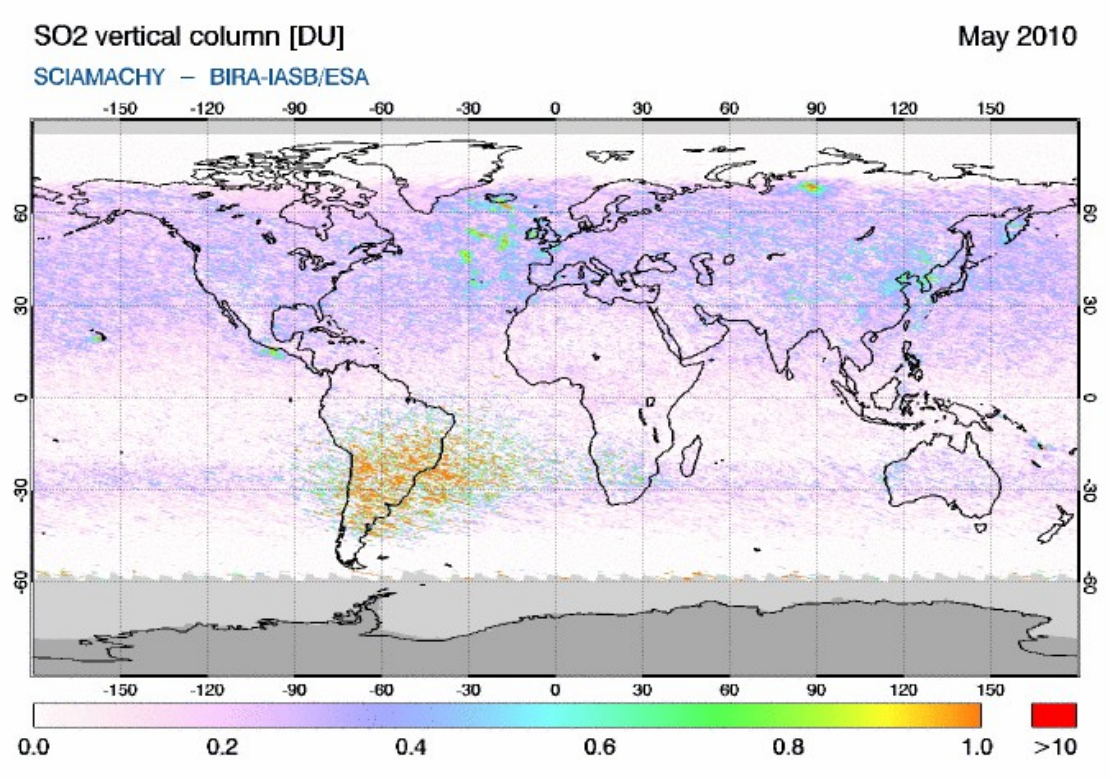

Figure 1

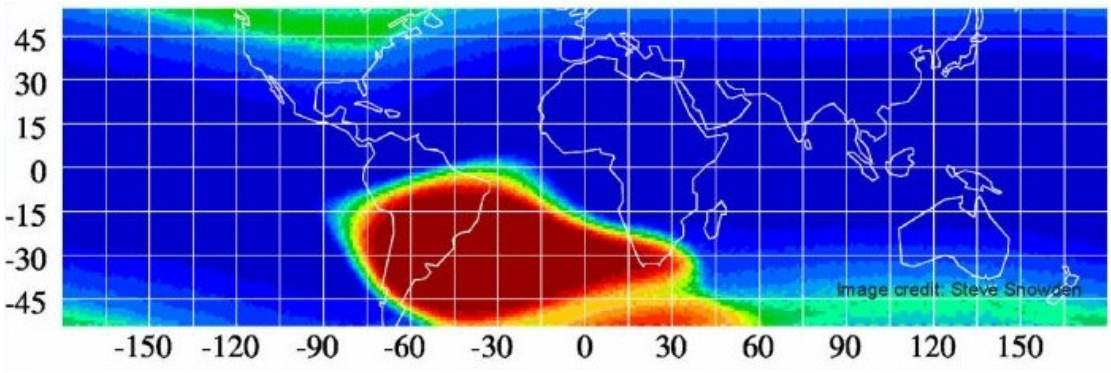

Figure 2

Figure 4 is an image of the South Atlantic Anomaly from data collected by the X-ray detector of ROSAT; it is taken from the ROSAT page on the SAA (http://heasarc.gsfc.nasa.gov/docs/rosat/gallery/display/saa.html).

4.2 Data quality assessment

In the frame of the O3M SAF project, an initial validation of the GOME-2 SO2 total column product (very similar to SCIAMACHY SO2 product in the processing approach) has been undertaken. In this study, the GOME-2 and SCIAMACHY SO2 columns results have been intercompared for different conditions: stratospheric plume (Kasatochi eruption), low-level SO2 plume (Kilauea eruptions on Hawai), and polluted boundary layer (Beijing). In general the comparisons show a good agreement for volcanic SO2: the locations of the peak SO2 values and the dimensions of the SO2 cloud match nicely. The differences in maximum SO2 columns can for a large part be explained by the use of different cross-sections at different temperatires in the DOAS retrieval. However, the satellite measurements of anthropogenic SO2 in the boundary layer have much larger uncertainties.
In a second step, the SCIAMACHY (and GOME-2) SO2 columns have been compared with ground-based MAX-DOAS (at Beijing) and Brewer (at Uccle and Manchester) measurements. In polluted region, the satellite observations are and MAX-DOAS observations (Beijing) are in reasonable agreement, but the uncertainties are large. For volcanic SO2, the passing of the plume from theKasatochi eruption over Europe has been measured with Brewer spectrometers in Uccle and Manchester. Comparisons of the Brewer measurements with satellite measurements show a very good agreement. Both the SCIAMACHY (and GOME-2) and the Brewer measurements capture the enhanced SO2 columns over Uccle and Manchester very well.

Details on this validation study can be found at:
http://o3msaf.fmi.fi/docs/vr/Validation_Report_OTO_SO2_Nov_2008.pdf