

<h1 style="text-align: center;">Volcanic & Air Quality SO₂ Service</h1> <h2 style="text-align: center;"><i>Product Information</i></h2>	 
<p><i>Document date:</i> 15 January 2008 <i>Data & Service version:</i> 1.0.3, S-07</p>	

Introduction

Sulphur dioxide (SO₂) enters the atmosphere as a result of both natural phenomena and anthropogenic activities, such as fossil fuel combustion, oxidation of organic materials in soils, volcanic eruptions and biomass burning. SO₂ contributes to acid rain and it is a key precursor for sulphuric acid aerosol formation. At high concentration, it also adversely affects human health, in particular in combination with fog (smog).

Changes in the abundance of SO₂ have an impact on atmospheric chemistry and hence on air quality and on climate. Effects of volcanic eruptions may have an impact on air traffic, as such eruptions are important sources of ash (aerosols) and SO₂. Consequently, global observations of SO₂ are important for atmospheric and climate research, and for air traffic organisations. Global monitoring of SO₂ concentrations is done on the basis of UV-Visible measurements by satellite based nadir-viewing instruments.

Volcanic emissions and strong pollution events are clearly detected with this approach, which makes it very suitable for use in a Near-real time (NRT) service, with an automatic Notification (or: Alert) Service for exceptional SO₂ concentrations. In addition to that an off-line (reprocessed) archive of data is useful for validation of the Service and the data, and for case studies of past events.

The SO₂ Services described here are closely linked to the so-called Support to Aviation Control Service (SACS) (<http://sacs.aeronomie.be/>) of the PROMOTE project. Apart from the SO₂ data, SACS also intends to deliver a volcanic ash indicator (VAI) as well as backward and forward trajectories from the location of an SO₂ peak value in case of an SO₂ alert. The trajectories are meant to indicate the possible origin and future motion of the SO₂, and the VAI is meant to provide additional information on possible volcanic eruptions.



The on-line product information

These web pages provide background information on the various aspects of the Volcanic & Air Quality SO₂ Service set up to monitor SO₂ emissions in NRT and off-line reprocessing, based on UV measurements made by several instruments based on different satellites.

Currently in use are SCIAMACHY (aboard ENVISAT) and OMI (aboard EOS-Aura). Later will follow data based on GOME-2 (aboard MetOp). Also a reprocessing of old GOME-1 (aboard ERS-2) data for the archive is planned.

The Services are set up using data from SCIAMACHY and so the product information is written from that starting point. Most information is, however, valid for the data of all instruments used -- if this is not the case, it is mentioned explicitly.

SO₂ data products

The technique used to retrieve the SO₂ slant column density from GOME-1, SCIAMACHY and GOME-2 data is the Differential Optical Absorption Spectroscopy (DOAS). From the slant column, the vertical or total column can be derived in two ways. One approach is to use an air-mass factor based on realistic SO₂ profiles. The other approach is to assimilate the slant column data in the chemistry-transport model TM; this approach is currently not in use. SO₂ data based on OMI is derived in a somewhat different way: with a "band residual method" using the residuals of the DOAS-based ozone retrieval.

The SO₂ column **archive service** provides global maps (monthly, 3-day composite [SCIAMACHY only] and daily) and global orbit data files. Higher resolution maps over pre-defined regions covering areas of possible volcanic and anthropogenic sources of SO₂ are provided as well. In addition access to the data files is given.

The **near-real time service** provides maps of daily orbit data files only, as well as the orbit data files themselves (except for OMI, for which only maps are presented).

Other data products

The volcanic ash indicator is based on observations of the SEVIRI instrument (aboard the geostationary MSG) and provides data only for the volcanoes in the field of view of SEVIRI (Europe and Africa). A description of this data product can be found ... *to follow*

The forward and backward trajectories will be added and described in due time.

Notes on this printed version

This is the printed version of the on-line product information on SO2 data derived from SCIAMACHY and GOMD for the Volcanic & Air Quality SO2 Service, part of the TEMIS and PROMOTE projects. A Table of Contents with page numbering can be found at the end of the document.

The latest version of the on-line product information can be found here
(<http://www.oma.be/BIRA-IASB/Molecules/SO2archive/info/>).

Links to other subjects within the product information are underlined in the printed version. Where links lead to other pages on the website, the phrase "[at the website]" is added, except for links to data files and such. External links are expanded.

This print is made using the "html2ps" software package from Jan Kärrman. Unfortunately the illustrations in this printed version are not so clear, due to the rendering of the images. Then again this document is not intended to be an official document, but merely to assist the user of the data. Official documents can be found in the "Documentation" section of the on-line product information.

Document date: 15 January 2008

Data version: 1.0.3

Service version: S-07

Author: Jos van Geffen

Websites: SACS (<http://sacs.aeronomie.be/>)

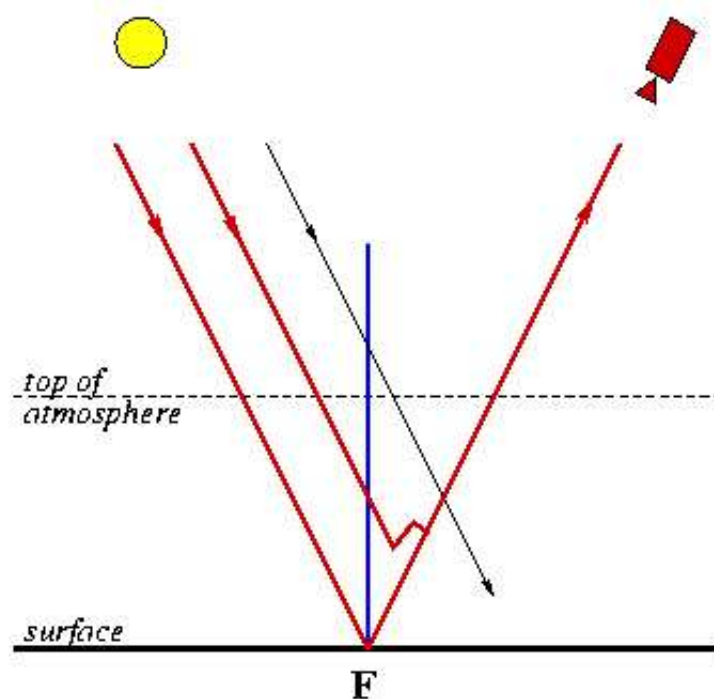
TEMIS (<http://www.temis.nl/>)

PROMOTE (<http://www.gse-promote.org/>)

Slant Column and Vertical Column Densities

Nadir-viewing satellite based instruments, such as GOME and SCIAMACHY, measure the sunlight scattered in the atmosphere and reflected by the surface of the Earth, as function of the wavelength of the light. In other words: the instruments measure earthshine spectra. Comparing such a spectrum with the spectrum of the sunlight itself provides information on the distribution and concentration of trace gases, such as ozone and SO₂, because these gases absorb or scatter part of the incoming sunlight. (Instead of using the solar spectrum for this comparison, one can also use an earthshine spectrum from a part of the atmosphere free of the trace gases under study.)

Cloud free case



*Schematic representation of the slant path (thick red lines) of incoming sunlight through the earth's atmosphere to the satellite, associated with the footpoint **F** (the point on the earth's surface the satellite is looking at). A part of the light reaching the satellite is reflected by the earth's surface, another part is scattered higher in the atmosphere. The thick blue line represents the "vertical column" at footpoint **F**.*

The above graph shows schematically the paths of sunlight reaching the satellite through the atmosphere, reflected by the earth's surface and scattered in the atmosphere. As the light follows these paths, some of the photons are absorbed by the trace gases in the atmosphere. The spectrum of the light measured by the satellite (the sum, as it were, of the thick red lines in the graph) thus provides information on the trace gases *along the entire light path*. In other words, the total density of a given gas, such as SO₂, is the concentration of this gas along the entire path. This is usually called the *slant column density* (SCD) associated with footpoint **F**, the point on the earth's surface the satellite is looking at.

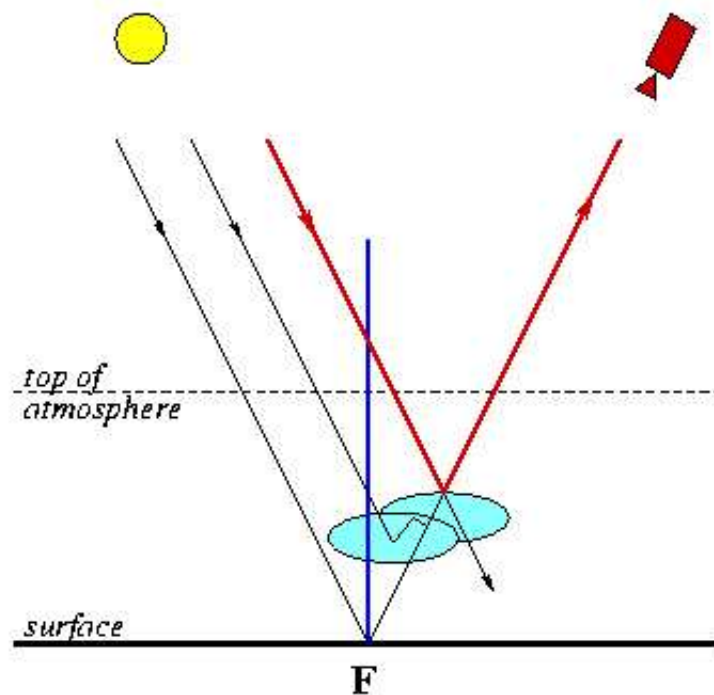
The SCD clearly does not provide the total concentration *right above* footpoint **F**, *i.e.* along the blue line in the graph. The total concentration along this line is called the *vertical column density* (VCD). It is this VCD that provides the most useful and directly interpretable information on the distribution and concentration of trace gases. It is therefore desirable to convert the SCD into the VCD.

As can be seen from the graph above, the VCD (along the blue line) is usually smaller than the SCD (along the red lines). The ratio between these two column densities:

$$\text{AMF} = \text{SCD} / \text{VCD}$$

is called the *Air-Mass Factor*. The value of the AMF depends on the length of the light path, the vertical distribution of absorbing trace gases in the atmosphere, the reflectivity (albedo) of the earth's surface, etc. The length of the light path depends on the position of the Sun (expressed in the Solar Zenith Angle, SZA) and the angle under which the satellite is looking at the atmosphere. The AMF can be pre-calculated for a variety of these quantities or computed with a chemistry transport model, and applied to the SCD to find the VCD at footpoint **F**.

Partly clouded case



*Schematic representation of the slant path (thick red lines) of incoming sunlight through the earth's atmosphere to the satellite, associated with the footpoint **F** (the point on the earth's surface the satellite is looking at), in the presence of clouds. These clouds partly shield the satellite's view of the atmosphere above footpoint **F**.*

If there are clouds in the atmosphere, things become more complicated. Clouds namely reflect (and scatter) incoming sunlight and thus effectively shield all that is going on below the clouds from the satellite's view. Clearly, the satellite measurements provide an SCD which contains only information on the atmosphere *above* the clouds. To find the real VCD at footpoint **F** in such situations, an "effective" AMF is computed, taking the cloud fraction (which gives the percentage of the cloud

cover) into account. In the presence of clouds the VCD is clearly less accurate than the VCD derived under clear-sky conditions.

There are two approaches possible to convert the SO₂ slant column density, retrieved with a DOAS technique, into a vertical column density. Both of these approaches use an air-mass factor (AMF), and they are described elsewhere in these pages:

- The use of a radiative transfer model to determine look-up tables.
- The use of a chemistry transport model, driven by up-to-date meteorological fields.

Geographic regions monitored in the Services

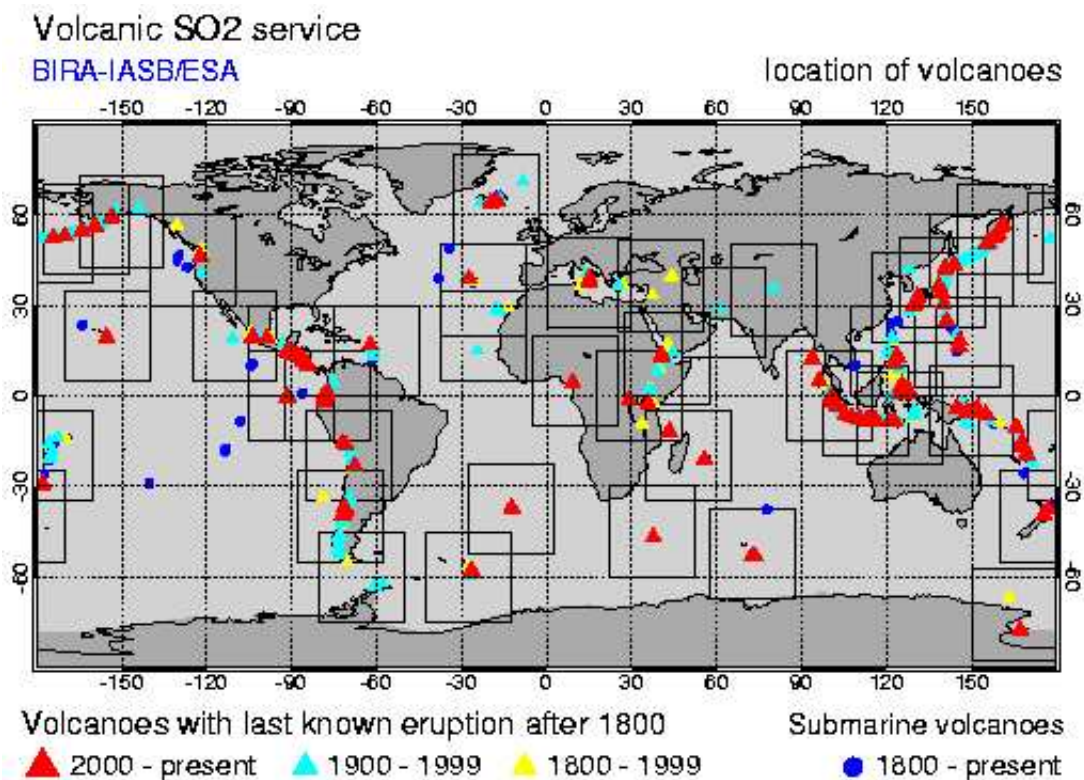
The SO₂ column values are presented and delivered via the website in the form of images (maps) and data files. There is no real difference between the Volcanic SO₂ and the Air Quality SO₂ Service, other than that they focus on different geographic regions. The Notification (or: Alert) Service or exceptional SO₂ concentrations of the Near-Real-Time (NRT) delivery monitors each of these regions.

The size of the regions is determined on the one hand by the wish to zoom in on sources of SO₂ emissions and on the other hand by the geographical coverage achieved by the satellite instruments when passing through the region: at least one orbit should pass through a region at any day.

The regions of the two Services partly overlap one another, which means that SO₂ emissions may be detected by both Services. As the measurement itself cannot distinguish between possible sources of SO₂ anyway, this is not a big problem.

In addition to plots for the individual regions of both services, two more plots are shown: one of the whole world shown in a cylindrical projection, and one which shows the two poles from above.

Volcanic SO₂ Service

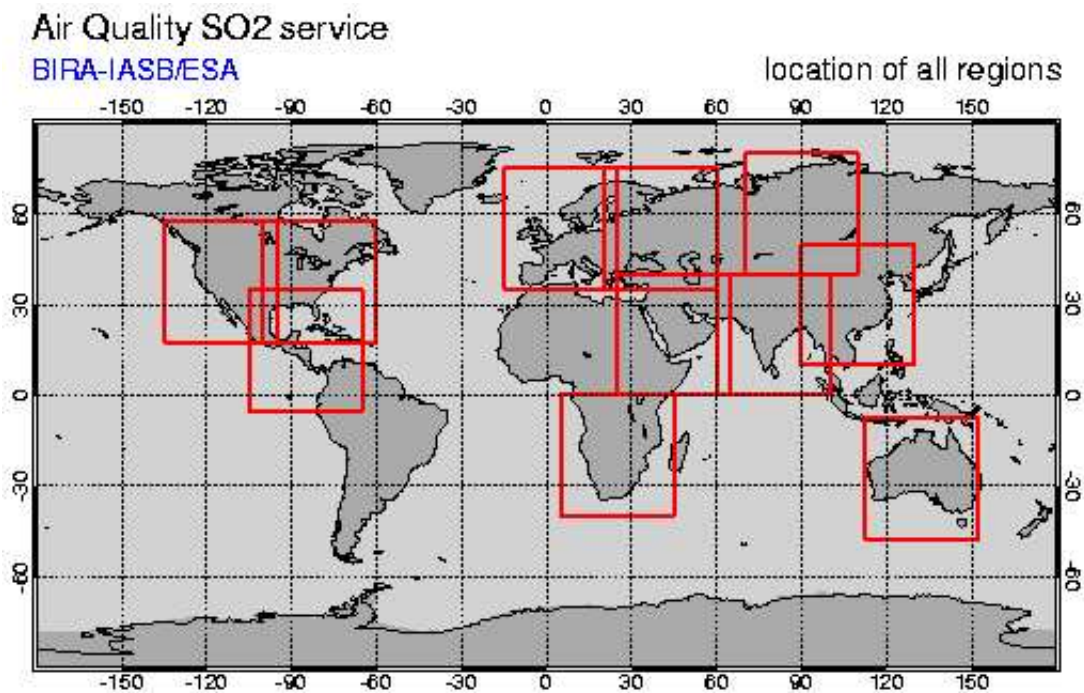


For the Volcanic SO₂ Service, a set of 42 geographic regions of 30 by 30 degrees covering known volcanoes has been defined. On the plots of the regions shown on the website, only shows the volcanoes in that region that have erupted since the year 1800, as listed on the website of the Global Volcanism Programme (GVP) (<http://www.volcano.si.edu/>).

The regions partly overlap one another, to ensure that SO₂ emissions from volcanoes near the edges of the regions are detected, whatever the wind direction.

See the [Overview of the Volcanic SO₂ Service regions](#) [at the website] for details.

Air Quality SO₂ Service



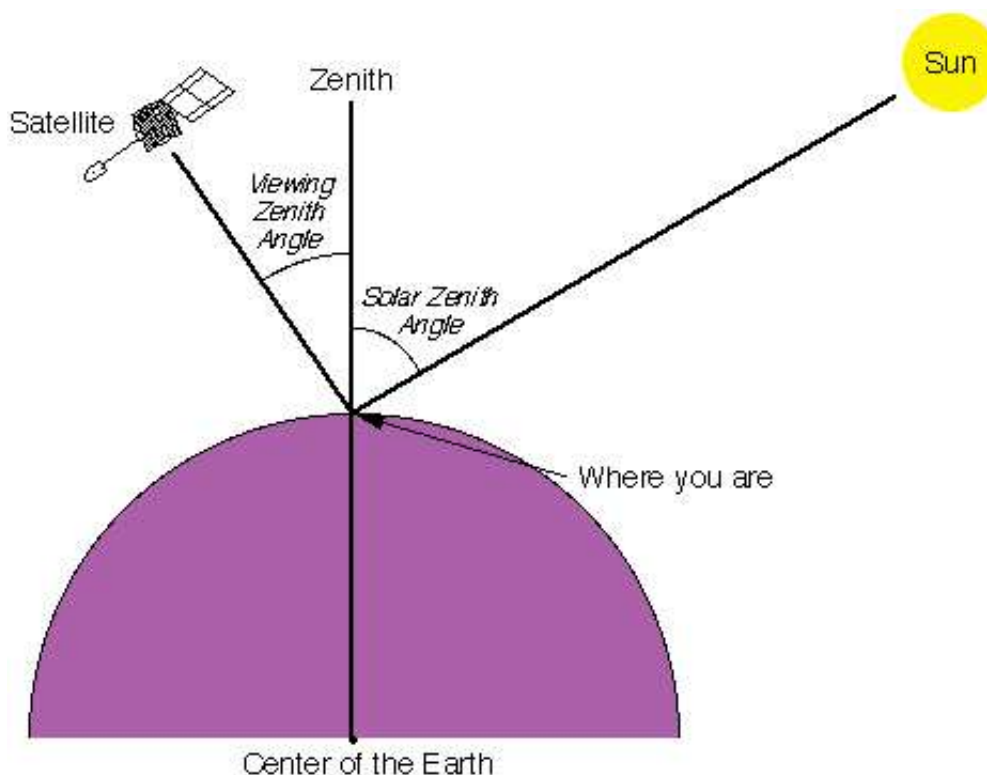
For the Air Quality SO₂ Service, a set of 11 geographic regions of 40 by 40 degrees covering industrialised areas has been defined.

There is no region defined for this Service over Southern America, because of the detection problems associated with the [South Atlantic Anomaly](#).

See the [Overview of the Air Quality SO₂ Service regions](#) [at the website] for details.

Solar Zenith Angle (SZA)

When observing a given point on the Earth's surface from a satellite-based instrument, the Solar Zenith Angle (SZA) is the angle between the local zenith (i.e. directly above the point on the ground) and the line of sight from that point to the sun. This means that the higher the Sun is in the sky, to lower the SZA is. The other angle in the graph, the angle between the local zenith and the line of sight to the satellite, is called the Viewing Zenith Angle.

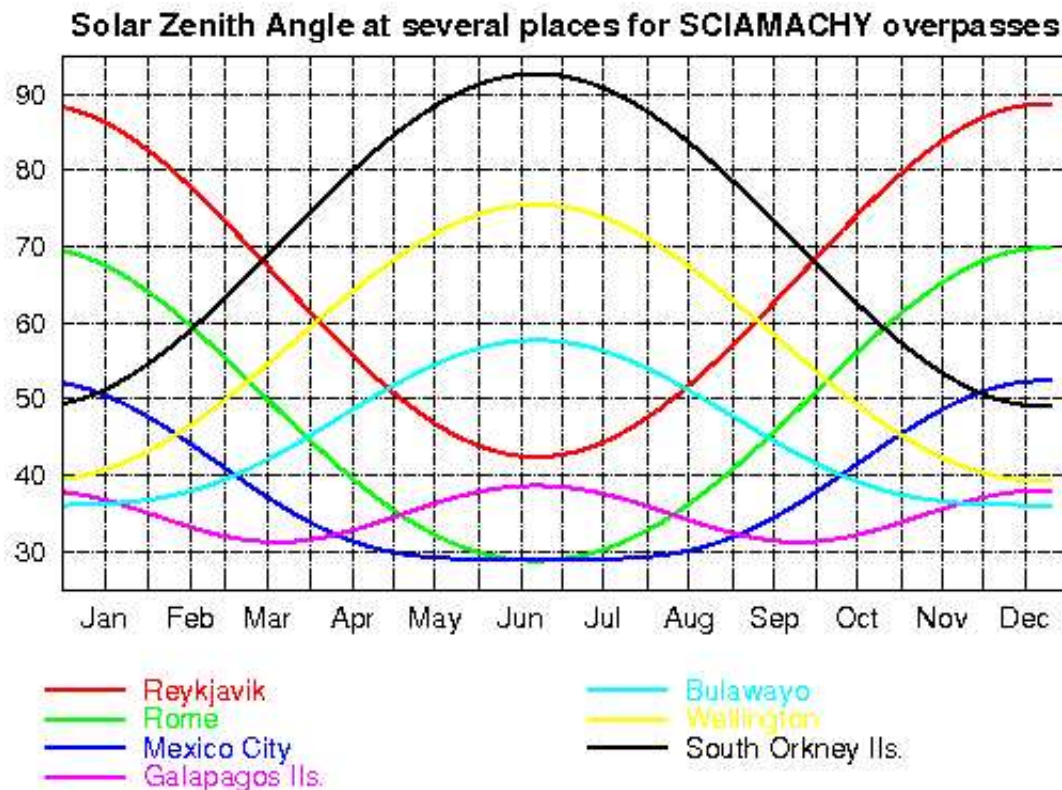


Schematic illustration of the Solar Zenith Angle (SZA) and Viewing Zenith Angle (VZA) for observations from satellite-based instrument.

[image taken from a [NASA page with definitions](http://asd-www.larc.nasa.gov/SCOOOL/definition.html) (<http://asd-www.larc.nasa.gov/SCOOOL/definition.html>)]

The value of the Solar Zenith Angle depends on the position on the Earth and the local date and time. The following graphs show the variation of the SZA for places at about the time SCIAMACHY passes directly overhead. The retrieval of SO₂ data is not so reliable for very high SZA, say above 75 degrees, and becomes really unreliable at much higher SZA. That is why data presented in the maps and data files on this website is limited to SZA 85 degrees.

The time SCIAMACHY passes a place overhead is always the same local time, as the satellite orbits the Earth in a so-called sun-synchronous orbit. If a satellite in a polar orbit flies over the pole into the sunlight, the SZA can be well above 100 degrees. The minimum SZA along the centre of an orbit is about 24 degrees. While orbiting on the sun-lit side of the Earth from North to South, SCIAMACHY scans from East to West, with on the East (West) side an SZA that is a little smaller (larger) than in the centre of the orbit.



The Solar Zenith Angle as function of time in 2007 for several places at about the moment SCIAMACHY passes overhead.

<i>place</i>	<i>latitude</i>	<i>longitude</i>	<i>time (UTC)</i>
Reykjavik	64.15	-21.97	ca. 12.35
Rome	41.88	12.50	ca. 09.40
Mexico City	19.40	-99.15	ca. 16:55
Galapagos IIs.	-0.50	-91.20	ca. 16:00
Bulawayo	-20.17	28.72	ca. 07:50
Wellington	-41.28	174.78	ca. 21:55
South Orkney IIs.	-62.00	-45.00	ca. 12:00

Note that ENVISAT, the satellite that carries SCIAMACHY, passes the equator at 10:00 a.m. local solar time. For a given longitude the time in UTC is:

$$\text{UTC_time} = \text{local_solar_time} - \text{longitude}/15$$

For example the Galapagos Islands are at about the Equator at 90 degrees West. With local_solar_time of 10:00 this gives a UTC_time for the overpass of about 16:00.

The following table lists the time and direction of equator passes of the different polar-orbiting nadir-viewing satellite instruments measuring SO₂. All these satellites have a sun-synchronous orbit at about 790 km above the surface.

<i>instrument</i>	<i>satellite</i>	<i>equator pass</i>	
		<i>local solar time</i>	<i>flight direction</i>
GOME-1	ERS-2	10:30 UTC	N -> S
SCIAMACHY	ENVISAT	10:00 UTC	N -> S
OMI	EOS-AURA	13:45 UTC	S -> N
GOME-2	MetOp-A	09:30 UTC	N -> S

What is the Dobson Unit (DU)?

The concentration of a certain trace gas, for example ozone and SO₂, in a column of air in the earth's atmosphere is often given in Dobson Units.

The "Dobson Unit" is named after professor G.M.B. Dobson (1889 - 1976), who has from the 1920s onwards done research on the ozone layer. Around 1930 he built the first "Dobson spectrophotometer", with which reliable measurements of the ozone layer became possible.



The "Dobson Unit" indicates how much of a given trace gas there is in the air above a certain point on earth. A proper unit in the International System of units would thus be "kilogram per square meter".

The unit introduced by Dobson is defined as follows. Suppose that all the trace gas in question in the air would be in a (gas) layer just above the ground, at standard pressure (1013.25 hPa) and at standard temperature (0.0 Celsius). The amount of the trace gas, for example ozone, is then indicated by the thickness of this layer, expressed in 0.01 millimeter. (This is why the ozone layer is sometimes referred to as being "thick" or "thin".)

1 Dobson Unit (DU) is:

- 2.6867E+20 molecules per square meter
- 4.4615E-04 MOL per square meter
- 2.1415E-05 kilogram of ozone per square meter

Averaged over the entire world the ozone column has a value of about 300 DU. For the Netherlands this is an average of 280 DU in autumn and 380 DU in spring. During spring on the southern hemisphere, September-November, the so-called "ozone hole" develops, with ozone values (well) below 200 DU.

For SO₂, the typical background level concentration (*i.e.* away from emissions related to pollution and volcanic eruptions) is much less than 1 DU. Emissions related to pollution and small volcanic eruptions are of the order of 1 DU or a few DU. Strong and explosive eruptions may lead to concentrations well above 10 DU, even as high as 100 DU.

Volume mixing ratio

Trace gas concentrations at a particular pressure level in the atmosphere are often given as a volume mixing ratio, or simply mixing ratio. This unit is defined as the ratio of the number density of the gas to the total number density of the atmosphere. In other words, the SO₂ volume mixing ratio is the density of SO₂ divided by the density of all constituents of the atmosphere in a unit volume (*i.e.* the number of molecules per unit volume).

Therefore, an SO₂ mixing ratio of 10E-09 means that the number density of SO₂ is 10E-09 times the total number density of air in a unit volume. Following the standard convention for the earth's troposphere and stratosphere, this mixing ratio equals 1 ppbv (parts per billion by volume).

For examples how to convert ozone volume mixing ratios into other units or vice versa, see [this page](http://wdc.dlr.de/data_products/SERVICES/PROMOTE_O3/vmr.html) (http://wdc.dlr.de/data_products/SERVICES/PROMOTE_O3/vmr.html) elsewhere on the Web.

Presentation and delivery of the data

The SO₂ column values, usually given in Dobson Units (DU), are presented and delivered via the website in the form of images (maps) and data files. Note that for OMI the NRT data files are not available; off-line OMI data is available via the NASA website.

There is no real difference between the Volcanic SO₂ and the Air Quality SO₂ Service, other than that they focus on different geographic regions. For each of the regions and for the world as a whole images are provided for the different data products. The data files always contain the data for the whole world. In all cases data is presented for solar zenith angles (SZAs) up to 85 degrees. Data of OMI is not limited in SZA.

This page gives an overview of the ways the data can be accessed and what is presented there:

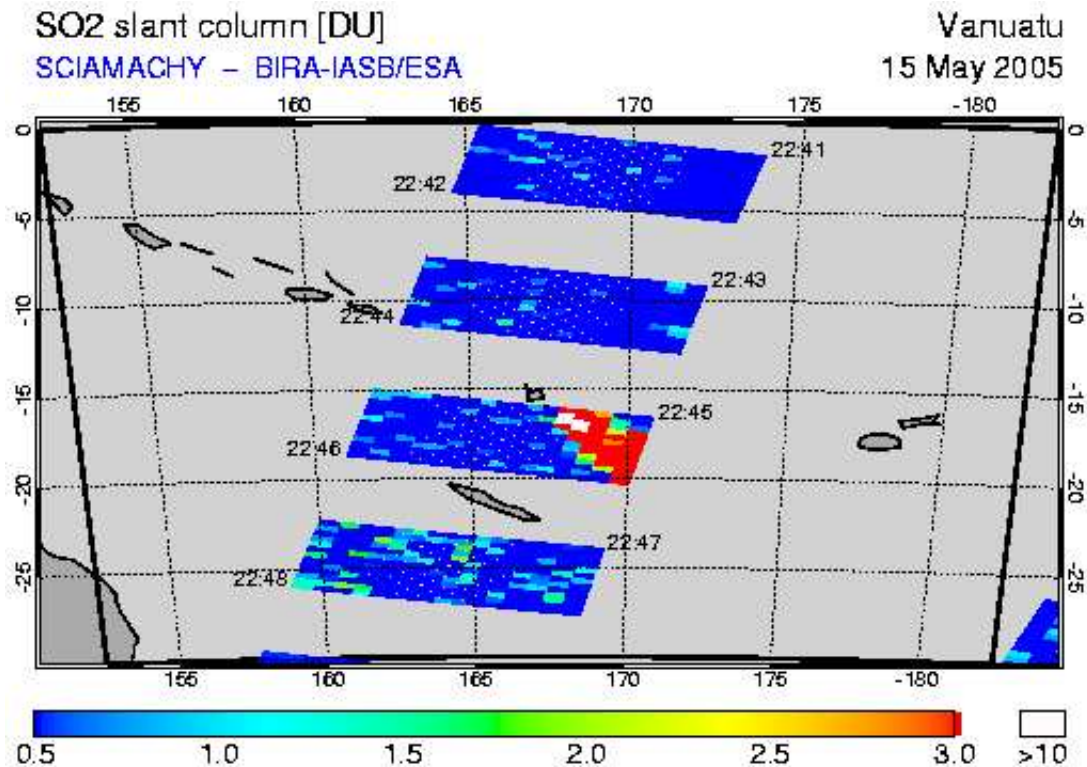
- [Daily data at orbit coordinates](#)
- [Daily data at grid coordinates](#)
- [Three-day composite data at grid coordinates](#)
- [Monthly average data at grid coordinates](#)
- Some further notes regarding the presentation and delivery of the data are given on a [separate page](#)

The following table lists for the different polar-orbiting nadir-viewing satellite instruments measuring SO₂ the normal swath width of the instruments and the size of their normal ground pixels within that swath.

<i>instrument</i>	<i>satellite</i>	<i>swath width</i>	<i>ground pixel size</i>
GOME-1	ERS-2	960 km	320 x 40 km
SCIAMACHY	ENVISAT	960 km	60 x 40 km
OMI	EOS-AURA	2600 km	12 x 24 km
GOME-2	MetOp-A	1920 km	80 x 40 km

The orbits of GOME-1 achieve global coverage at the equator in three days. SCIAMACHY would also have global coverage in three days if only it were not for the alternating between nadir and limb viewing (only the nadir viewing measurements can be used here; cf. the example plots shown below). Due to its wide swath with OMI achieves global coverage in one day. The swaths of GOME-2 are just a little too small for complete global coverage at the equator in one day, but the gaps between successive orbits are small.

Daily data at orbit coordinates



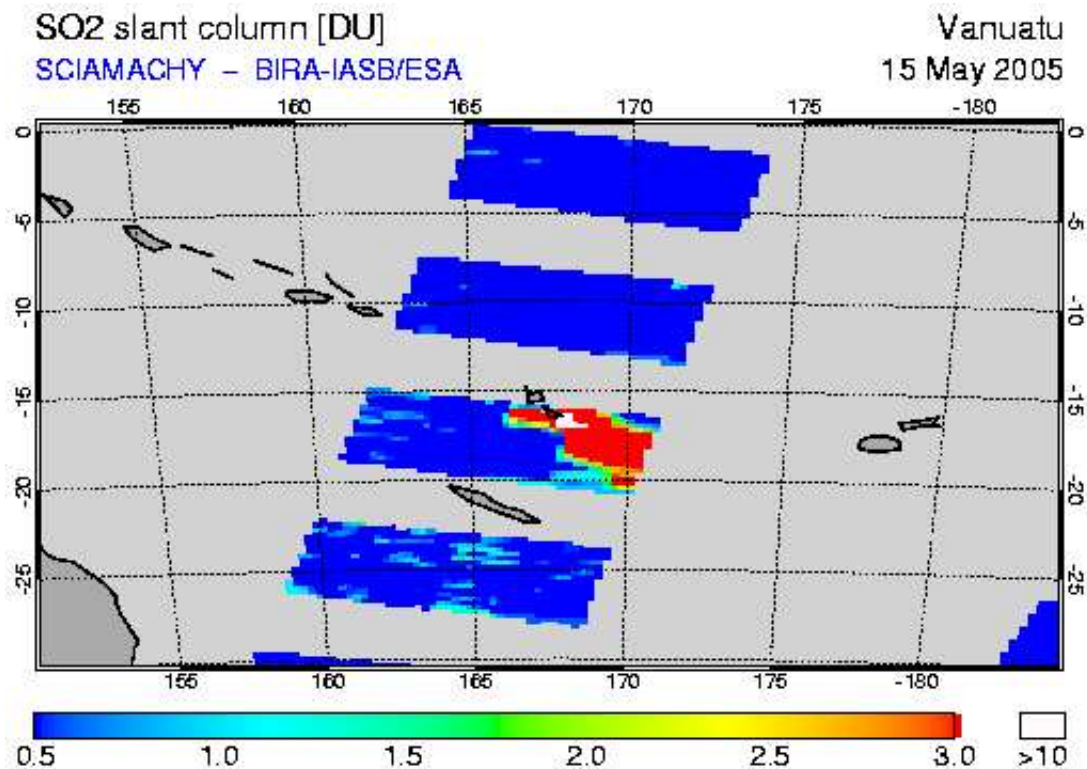
This presents the SO₂ data at the coordinates of the measurements of the satellite instruments. Note that at high latitudes the scans of successive orbits will overlap one another, where the most recent data is plotted on top.

In pictures based on data from scanning instruments (GOME and SCIAMACHY) only the forward scan pixels are shown; backward scan pixels are not shown to prevent overlapping. In OMI pictures all data is shown, since OMI is an imaging rather than a scanning instrument.

In SCIAMACHY pictures, at the begin and end of each nadir state the measurement time is shown. In OMI pictures the measurement time of a given swath is printed in the middle of the swath. Times are always in UTC. Note that the time is not printed for states with latitudes above ± 65 degrees, as orbits overlap one another there. For the Volcanic SO₂ Service, the extent of the geographic region is indicated by a thick black line.

Both the NRT and the Archive Service provides data and images of the SO₂ vertical (total) column and the slant column, and the [cloud fraction](#). Each orbit has its own ASCII data file; for a given day these ASCII data files are grouped in a zip-file.

Daily data at grid coordinates



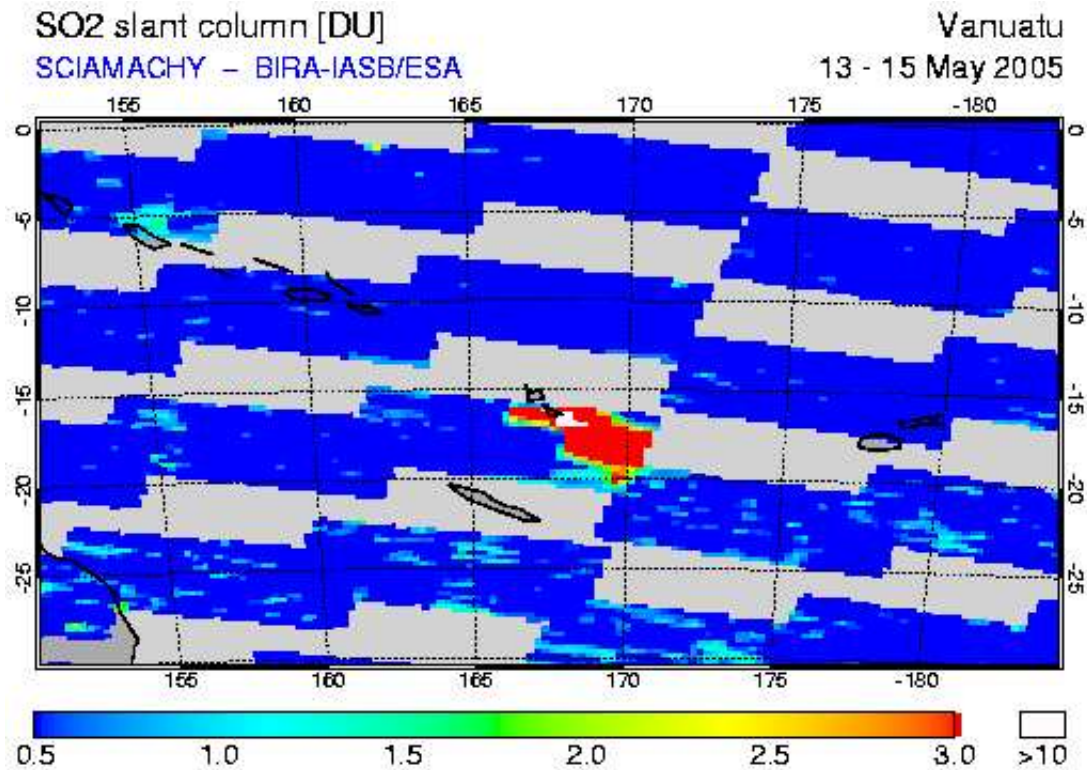
This presents the SO₂ data gridded to a latitude-longitude grid of 0.25 by 0.25 degrees (which is about 25 km at the equator). For each grid cell the average of all measurement crossing that grid cell (i.e. using both forward and backward scans in case of scanning instruments) is computed, using all orbit files for the given day. The result is written to one HDF data file per day.

The Archive Service provides such images for the SO₂ vertical (total) column and vertical column (if available), and where possible the cloud fraction. The Near-real time Service does not provide this type of data.

NOTE: it is not yet certain whether this time of data/images is going to be provided also for OMI and GOME-2 derived data.

Three-day composite data at grid coordinates

Only for GOME-1 and SCIAMACHY data, since these instruments do not have global coverage in one day.

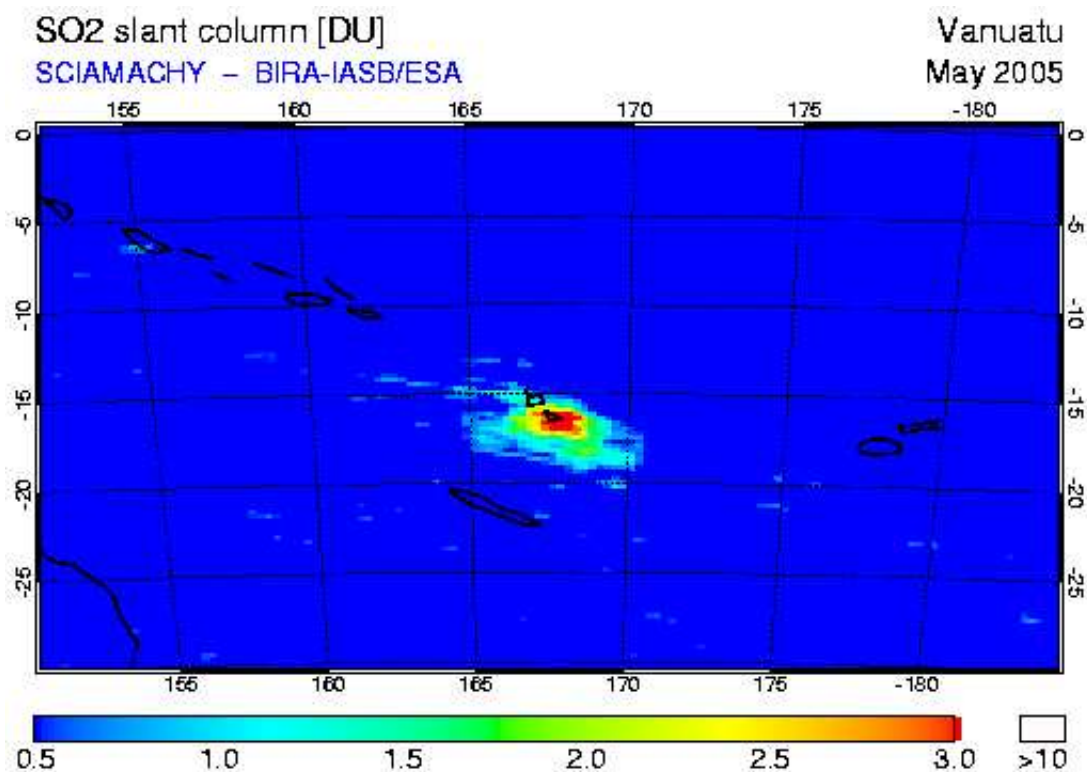


This presents the SO₂ data gridded to a latitude-longitude grid of 0.25 by 0.25 degrees. For each grid cell the average of all measurement crossing that grid cell (using forward and backward scans) is computed, using all orbit files for three days (01-03, 04-06, etc). The result is written to one HDF data file per three days.

In view of the width of the measurements (960 km), global coverage along the equator is reached in three days, hence the use of three-day composites. For GOME-1 this is real global coverage. For SCIAMACHY there are "holes" in the orbits due to the alternation between nadir and limb measurements, and these Services can only use the nadir measurements.

The Archive Service provides data and images for the SO₂ vertical (total) column and the slant column, and the cloud fraction. The Near-real time Service does not provide this type of data.

Monthly average data at grid coordinates



This presents the SO2 data gridded to a latitude-longitude grid of 0.25 by 0.25 degrees. For each grid cell the average of all measurement crossing that grid cell (using forward and backward scans) is computed, using all orbit files for the given month. The result is written to one HDF data file per three days.

The Archive Service provides data and images for the SO2 vertical (total) column and the slant column. The Near-real time Service does not provide this type of data.

Note that a monthly average of the cloud fraction is not made: there is no cloud screening method applied to the SO2 data, so that a monthly average cloud fraction does not provide any useful additional information.

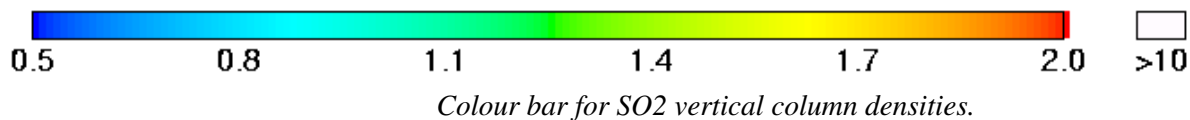
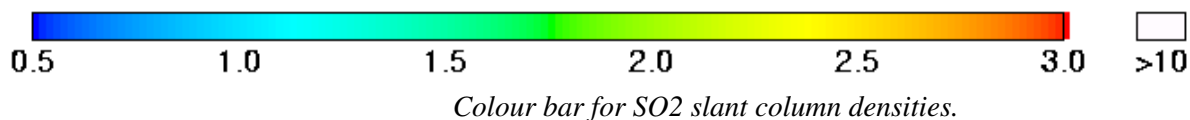
Presentation and delivery of the data -- some notes

Some notes regarding the [Presentation and delivery of the data](#):

- [The colour scale of the plots](#)
- [Plots of overlapping orbits](#)
- [Plots for the website made with IDL](#)
- [Date of the data files and the plots](#)
- Some notes on downloading the data are given on a [separate page](#)

The colour scale of the plots

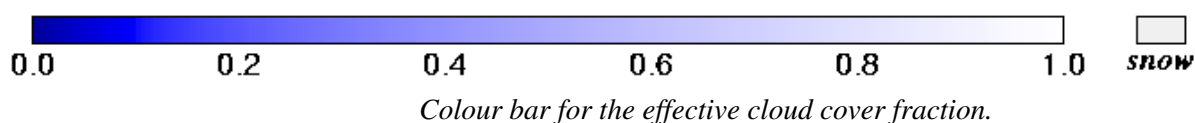
The colour scale of the SO₂ slant and vertical column plots shows the colour coding for the concentration in Dobson Units (DU). All values equal to and below 0.5 DU have the same colour (blue); the lower limit is set to this value to remove most of the noise due to the SO₂ background. The upper limit of the regular colour bar is different for the SO₂ slant columns (3.0 DU) and vertical columns (2.0 DU), since the slant column values are usually higher than the vertical column values. A special colour is used for really strong SO₂ signals -- usually these associated with volcanic eruptions -- with the same value for the slant and vertical column plots.



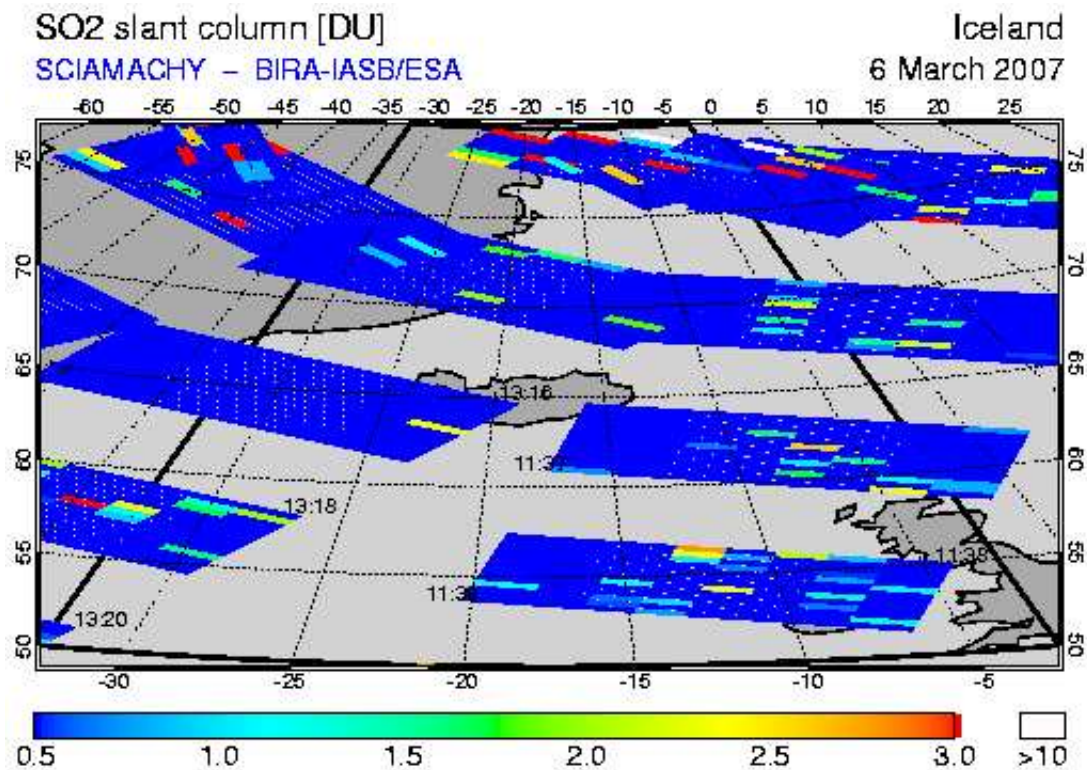
The reason to end the main scales at 2 and 3 DU is to make sure that low level SO₂ concentrations are visible, concentrations that can be great interest too, e.g. because they signify small-scale volcanic eruptions. Furthermore, it is most interesting to show where large concentrations of SO₂ appear, without being too specific about the exact values, especially because large SO₂ concentrations do not occur that widespread or that often. Furthermore, representing all data using the same colour makes it easy to compare results for different periods and regions.

Note that the scale for the SO₂ plots shown on the website varies linearly. For special purposes, however, the scale may have other ranges and/or may be logarithmic.

The colour scale of the (effective) cloud fraction varies linearly from zero (cloud free; dark blue) to one (fully clouded; white). Values below zero and above one cannot occur. The snow/ice mode of the cloud data products is represented by very light grey (indicated simply as "snow" in the colour bar).



Plots of overlapping orbits



At high latitudes, above 65 degrees or so, satellite orbits overlap since the swath width of the instrument has a fixed size at ground level (960 km in normal mode for GOME-1 and SCIAMACHY, about 2000 km for OMI and GOME-2). When plotting the daily data at orbit coordinates, this plotting is done with the orbits listing in ascending time. As a result, the values shown in the plot at a given location are those of the latest orbit of that day. This can be seen clearly in the SCIAMACHY-based picture shown here.

For the gridded data this is not a problem: all data falling in a given grid cell is averaged for that grid cell and therefore each grid cell has a unique data value.

Plots for the website made with IDL

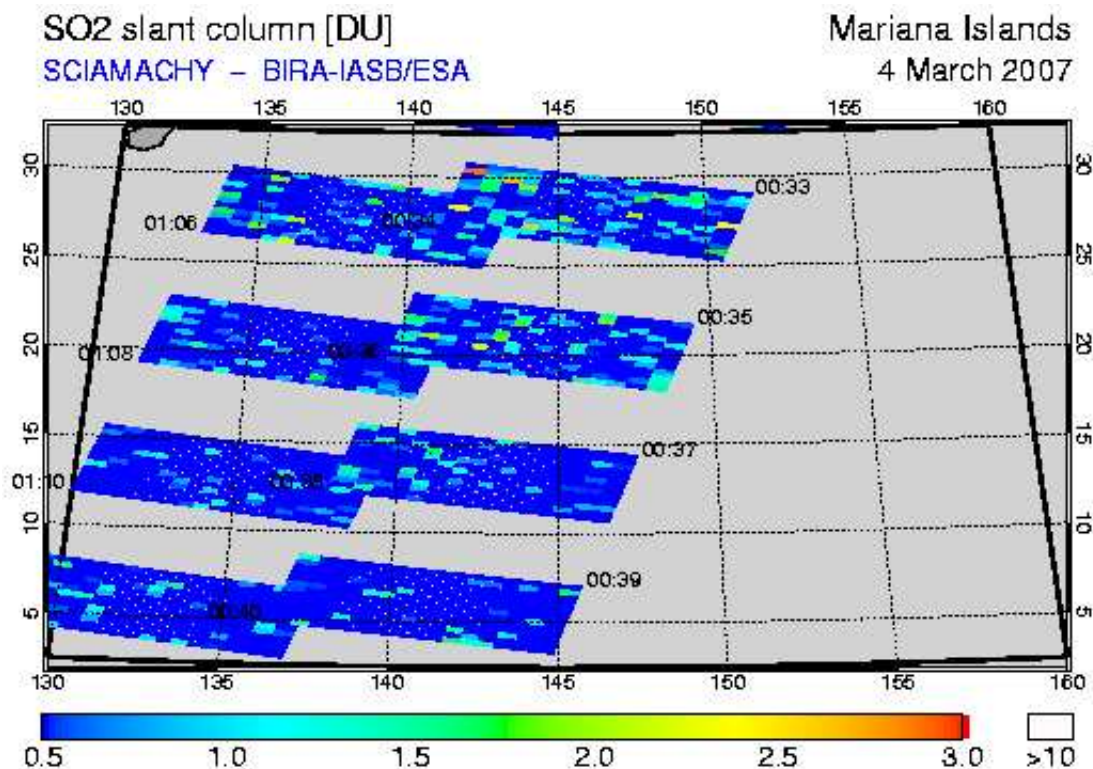
The plots of the SO₂ data and the associated maps are all made with IDL (version 6.3). Some notes:

- The IDL plotting routines include the possibility to draw lines along continents and to colour the continents. IDL appears to have some problems correctly colouring the continent Antarctica. The reason for this is that the information for colouring the continents and for drawing the borders is taken from two different databases, which evidently differ at the border of Antarctica. The line around the continents shows the real border.
- Unfortunately, the lakes drawn on the maps by IDL do not get the same colour as oceans do: lakes get the land colour, whereas one would expect lakes to have the sea (water) colour. This is especially clear in the plots of [Eastern Europe](#), where the Black and Kaspian Sea and several lakes are given the land colour.

- On the maps of the regions, boundaries of the countries are drawn. These boundaries are the political boundaries from 1993. IDL's database unfortunately does not have all borders correct; for example, in Arabia boundaries are missing. The IDL developers are aware of this problem.

For plots of the daily data at orbit coordinates, rectangles made up of the ground pixel corners as given in the data product are filled with the appropriate colour. Since these rectangles are made up of straight lines, they do not exactly match those north and south of them: there are little openings between the rectangles, because the earth's surface is curved. This can, for example, be seen in the example image shown above and below. It does not show up in the images of the gridded data.

Date of the data files and the plots



Data files are grouped together per day, where the date is determined by the *start time* of the given orbit. This means that if a given data file starts just before midnight of a certain day and continues into the next day, the plots of the day will also show some data from the next day. And similarly for the HDF files for the day.

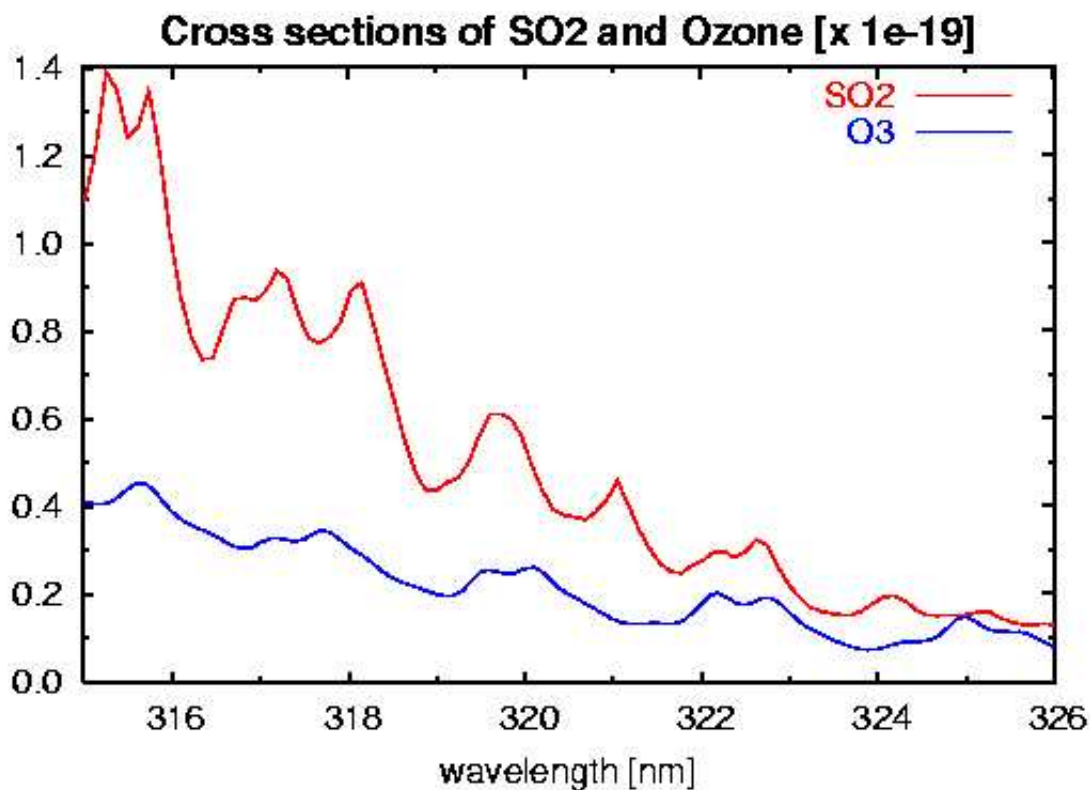
The image shown here gives, which uses SCIAMACHY data, an example of this for the date 4 March 2007. The states of the orbit on the left, with measurement times of about 01:08 UTC, are measured early on 4 March -- this is in fact the first orbit of that day, which started at about 00:11 UTC. The states of the orbit on the right, with measurement times of about 00:35 UTC, are measured early on the next day, 5 March: they are part of the orbit which started at about 23:40 UTC on 4 March.

SO₂ slant column retrieval

The SO₂ slant column density, usually given in Dobson Units (DU), are retrieved from UV measurements made by satellite based instruments, such as GOME-1, SCIAMACHY (in the nadir-viewing mode) and GOME-2. The retrieval method applied to the measurements of these instruments is the Differential Optical Absorption Spectroscopy (DOAS) technique.

SO₂ data based on OMI is derived in a somewhat different way: with a "band residual method" using the residuals of the DOAS-based ozone retrieval. More info and links can be found in the section on the SO₂ column from OMI.

The retrieval of the SO₂ slant column is done from the spectrum in the wavelength range 315-326 nm, where SO₂ shows clear absorption features. In the same wavelength range, however, there is also absorption by ozone (O₃). The retrieval must therefore take both SO₂ and O₃ into account. There is, so to say, an "interference" of the two absorption signals when matching the measured spectrum with the absorption cross sections of SO₂ and ozone.



Cross sections of SO₂ (red) and ozone (blue) in the wavelength range used for the SO₂ slant column retrieval.

The result of this "interference" is that when concentrations of SO₂ are low, the retrieval may give negative SO₂ slant column values, with an error of the same magnitude. This then represents the SO₂ background level, *i.e.* the apparent SO₂ absorption in the absence of emissions of SO₂. The negative values are, of course, not physical, but due to the fact that it is not possible to retrieve SO₂ independently from ozone.

For low Solar Zenith Angles (SZAs), *i.e.* at low and mid latitudes, the SO₂ background level is of the order of 1 Dobson Unit (DU) and emissions of SO₂ (by pollution or volcano eruptions) will be visible against this background.

For higher SZAs, however, there is a problem. The higher the SZA, the longer the slant path is along which the retrieval takes place. Because of the vertical and horizontal distribution of ozone in the atmosphere (with a strong concentration in the lower stratosphere, the "ozone layer") a longer slant path means a larger relative absorption by ozone. For SO₂ this is much less the case, as SO₂ emissions generally show a rather limited distribution horizontally and vertically.

Effectively this means that at higher SZAs the "interference" between the SO₂ and O₃ absorption results in more negative SO₂ slant column values, with large errors. This effect is corrected for by the background correction which is applied to the slant column data.

Slant column error

The data files delivered via the website contain the value of the slant column density (SCD) in Dobson Units and an estimate for the retrieval error on the SCD, also in Dobson Units. This error does *not* take into account any errors in the background correction, the air-mass factor, or other steps in the process: the error just reflects the error due to the DOAS retrieval of the slant column.

Slant column retrieval details

In the DOAS retrieval the following trace gases are fitted in the wavelength range 315-326 nm: SO₂ and ozone at two temperatures (223 and 243 K). Furthermore two Ring spectra are fitted to correct for the Raman scattering, one to account for the general Ring effect of the Fraunhofer, one for the contribution of ozone (which in fact depends on the solar zenith angle). In addition a correction for polarisation effects and a wavelength calibration using a high-resolution solar spectrum are performed.

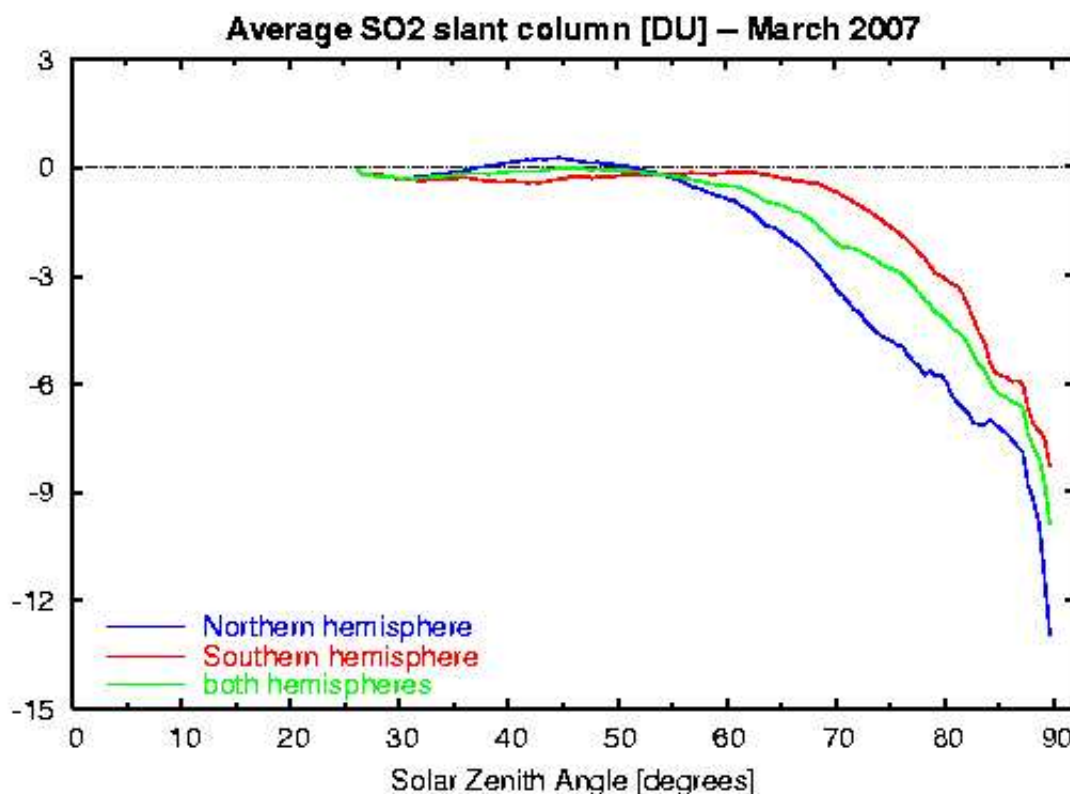
Background correction of the SO₂ slant column data

A background correction is applied to the SO₂ slant columns retrieved with DOAS based on satellite measurements. This section describes the correction as it is applied to SCIAMACHY data; for GOME-1 and GOME-2 the method will probably be similar (this is to be determined). For OMI data the background correction is done differently; see for info and links the section on SO₂ column from OMI.

There are two reasons to apply such a correction on the SCIAMACHY data:

- The DOAS retrieval requires the use of a reference spectrum. As reference spectrum for SCIAMACHY data a measurement is used from a location thought to be free of SO₂, but the retrieval can still lead to an offset (bias) in the SO₂ slant column.
- At higher Solar Zenith Angles the "interference" between the SO₂ and ozone absorption -- mentioned in the SO₂ slant columns retrieval section -- results in more negative SO₂ slant column values, with large errors.

The following graph shows an example of the monthly average SO₂ slant column as function of SZA.



Average of the SO₂ slant column as function of the SZA for March 2007 over all data (green), of only the Northern hemisphere (blue) and of only the Southern hemisphere (red). The decrease of the average SO₂ slant column at higher SZA is due to the increase in ozone absorption along the slant path with increasing SZA.

From this graph it is not only clear that the retrieved SO2 slant column decreases strongly at high SZA, but also that there is a difference between the Northern and Southern hemisphere here. The reason for the latter difference is that ozone concentrations near the South Pole are much lower than near the North pole due to the presence of the "ozone hole" above Antarctica in this month. This indicates that the correction for effects of the "interference" at high SZA should be a function relating the SO2 slant column with the ozone concentration.

The monthly average SO2 slant column represents the background level of SO2 in the retrieval: on average, there will be not much SO2 in the atmosphere, as SO2 emissions are highly localised and SO2 has a short lifetime in the atmosphere (in the troposphere up to a few days; in the stratosphere longer). Consequently, the average can be used to compensate for the offset (bias) caused by the use of the reference spectrum. This offset is clearly visible in the above graph for low SZA.

Correction for the offset

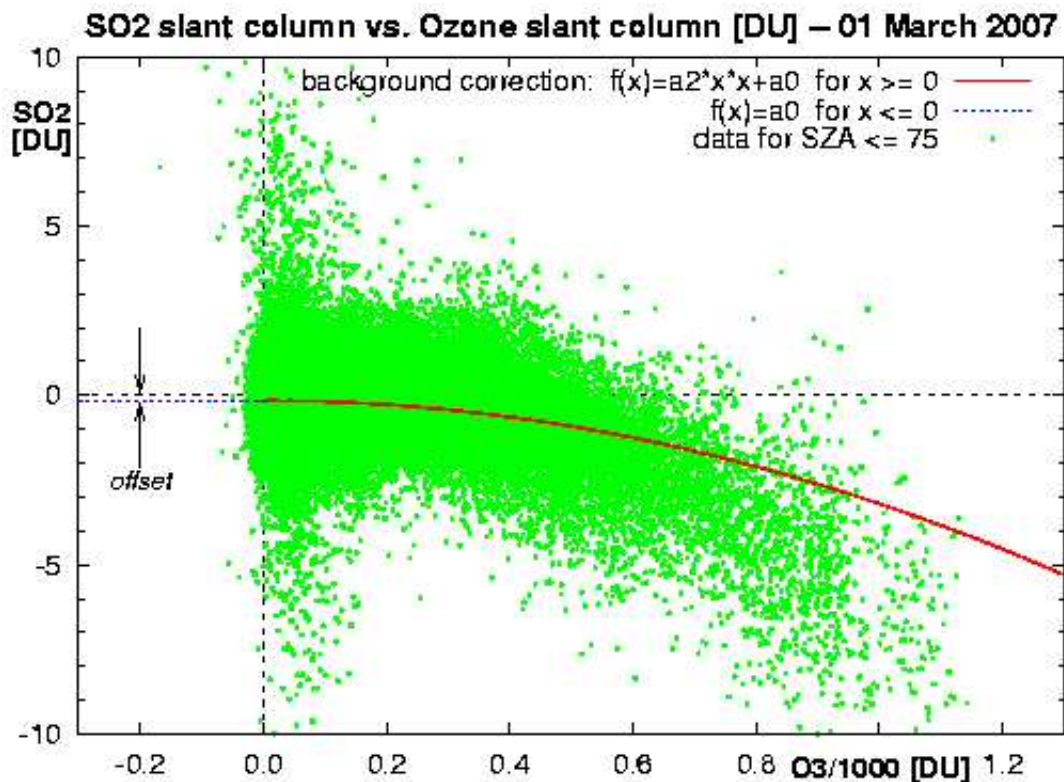
The monthly average SO2 slant column shows at low SZA an offset due to the use of a reference spectrum, which is changed once a month. To find the offset, all SO2 slant column values for SZA < 50 degrees are averaged, with the SO2 slant column error as weights in the averaging.

There may be large SO2 peak values that are real signals and these should therefore not be taken into account when computing the background that is assumed to be free of SO2. For that reason, once the above mentioned averaging gives the offset, another round of averaging is done of all the data that does not differ more than 5 DU from the average of the first round.

The average of the second round then gives the offset value to be used in the background correction.

Correction for the interference

To find the correction for the interference in the absorption signals at high SZA, a function is sought which relates the SO2 slant column against the ozone slant column value that is also given by the DOAS fit. Looking at the data points for SZA < 75 degrees for a given period of time indicates that this function is parabolic, as can be seen from the following graph for the data points of one single day.



The green dots in this graph are all data points of 1 March 2007 with SZA < 75 degrees, with the SO2 slant column in DU as function of the ozone (O3) slant column in units of 1000 DU. The arrows and the blue dashed line on the left indicate the offset ("a0") due to the use of a reference spectrum determined from an average of all data points from March with SZA < 50 degrees. The solid red curve is the parabolic function of the background correction that follows from all data points of two years (2005-2006).

The SO2 values at high ozone concentrations vary a lot from day to day and from month to month. Performing a parabolic fit through the data would then give different coefficients for different months, and these coefficients can vary really a lot (from -8 to close to zero). The reason for this large variation in the parabolic coefficient is that the number of data points for SZA > 50 degrees varies from month to month and is much smaller than for lower SZA.

The parabolic coefficient for the background correction, shown by the red line in the above figure, is based on a fit through all data points with SZA < 75 degrees for all days of two years: 2005 and 2006 (a total of 42.6 million points).

Again to avoid real SO2 peak values from influencing the fit, the fit is done in two rounds: first with all points, then again but omitting those points that have an SO2 slant column of more than 5 DU away from the parabolic curve.

The correction for the interference described above is working quite well, much better than the previous correction (see for a comparison below): in the Northern Hemisphere Spring -- when problems were biggest in terms of seemingly large SO2 concentrations at high SZA and consequently "false alerts" by the notification system for "exceptional SO2 concentrations" -- the number of such problem cases is reduced dramatically.

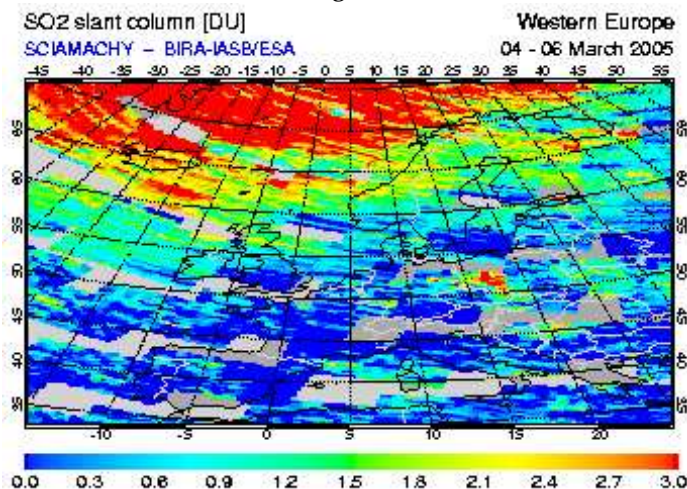
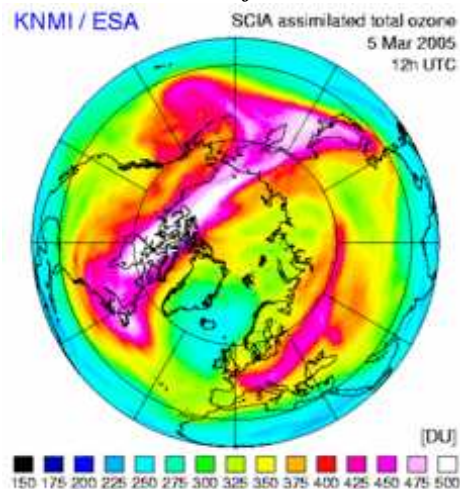
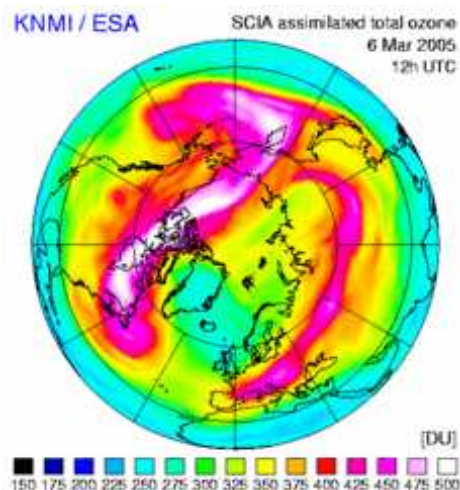
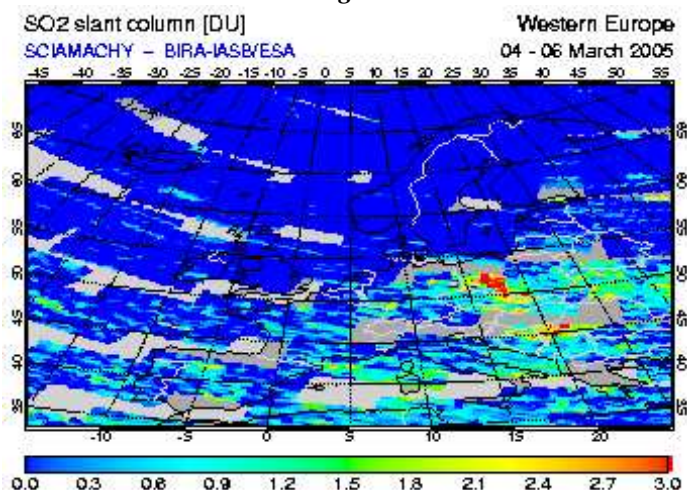
But the problems are not complete over yet, as described in a [special subsection](#). For the moment we do not know how we could set up a better correction of the interference problem and thus avoid problems these problems.

Improvement with the new correction for the interference

The drop on the SO2 slant column values at large SZA, due to the "interference" between the absorption signals of SO2 and ozone, was in a first attempt corrected by a function linking the SO2 slant column against the SZA. Doing that required different functions for the two hemispheres: the monthly average SO2 slant column for the two hemispheres can be quite different, as the above graph for October 2004 shows. In addition, each month requires a different function.

This approach -- applied up to [data version 0.9](#) -- worked reasonably well for most situation. But it appeared to fail for situations where the ozone concentration shows a strong variation in the longitudinal direction (in fact: along a line of equal SZA), as is often the case on the northern hemisphere in Spring, the correction does not work well. This lead to SO2 values strongly positive or strongly negative in situation where there is in reality no (or very little) SO2.

With the new background correction described above, the SO2 slant column values are much more reasonable, and there are far less extreme SO2 values. The improvement due to the new background correction can be seen clearly from, for example, in the following images.

SO₂ -- old background correction**ozone field****SO₂ -- new background correction**

The top-left image shows the three-day composite of the SO₂ slant column over Western Europe in early March 2005 based on an old (version 0.9) background correction. The large SO₂ values over the northern part of the Atlantic Ocean are unlikely to be realistic! They are most likely due to ozone values well below the average.

The bottom-left image shows the same three-day composite but now with the new background correction, described on this page. Clearly, the large SO₂ values over the northern Atlantic have all gone and the whole picture looks much more realistic.

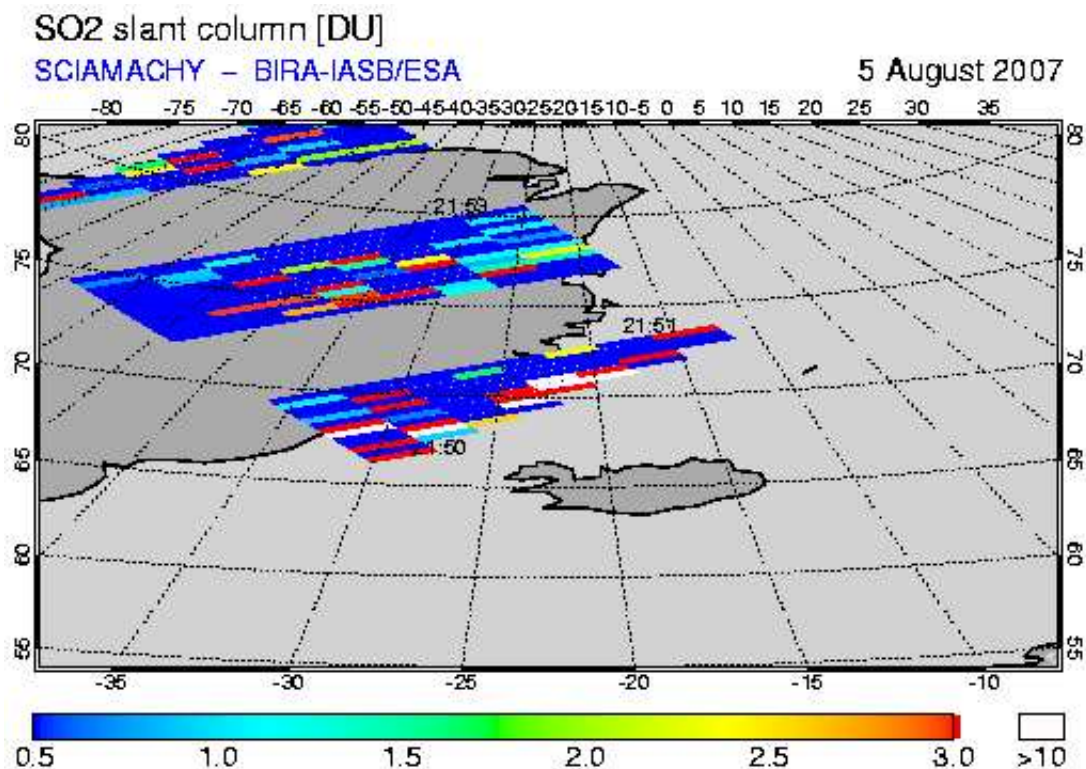
For the days of March of the SO₂ plots, the ozone value varies considerably along a given longitude, as can be seen from the images of the ozone field on the right for 5 March and 6 March (click to see the [ozone field for 4 March](#)).

[Ozone images taken from the archive of the [TEMIS global total ozone field](http://www.temis.nl/protocols/O3global.html) (<http://www.temis.nl/protocols/O3global.html>).]

Remaining problems with the correction for the interference

The correction for the ozone interference described in the [main background correction section](#) is working quite well, much better than the previous correction and the number of problem cases is reduced dramatically. But the problems are not complete over yet, as described below. For the moment we do not know how we could set up a better correction of the interference problem and thus avoid problems like those mentioned here.

Problems at high SZA

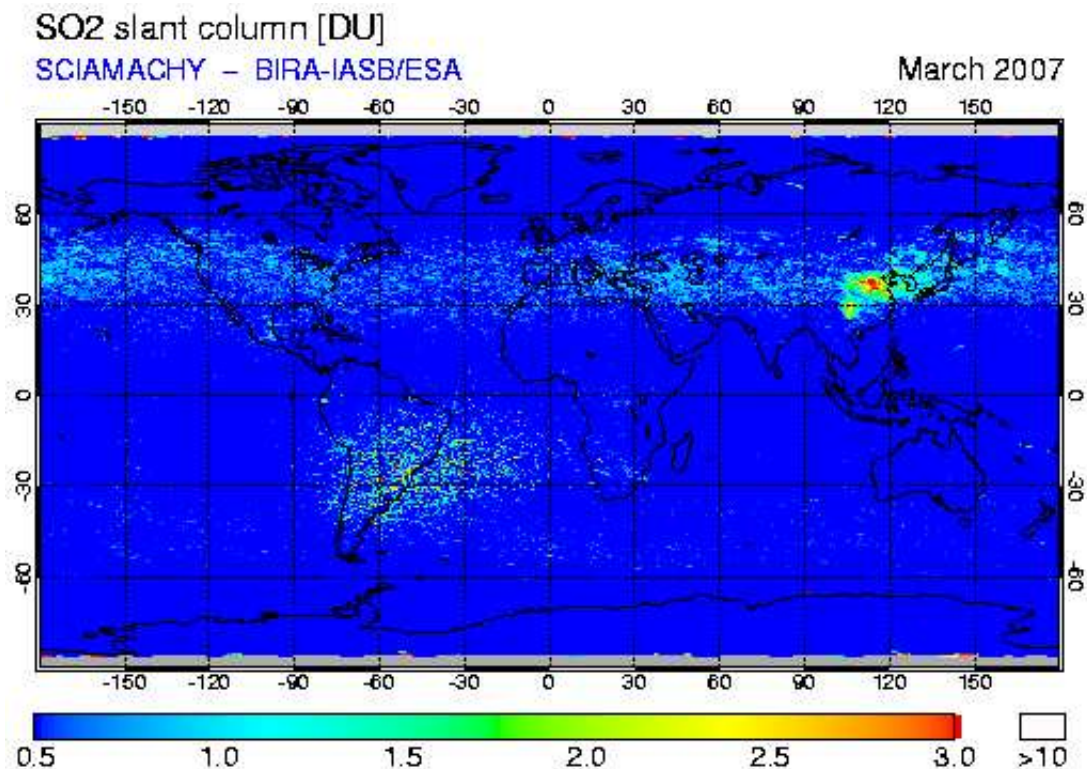


For SZA well above 75 degrees there can still be a problem, as the graph of the SO₂ slant column near Central Russia given here clearly shows: the nadir state in the middle near the top shows a few ground pixels with slant column values of more than 10 DU. There are no reports of volcanic activity on Iceland around that time, nor is there any anthropogenic source nearby. Clearly, the seemingly high SO₂ values in this graph are artifacts.

Note that the data is plotted only for SZA < 85 degrees and that the satellite moves in this graph towards the top-left part of the image: the nadir states shown are the beginning of an orbit that will cross the equator at about 175 degrees East.

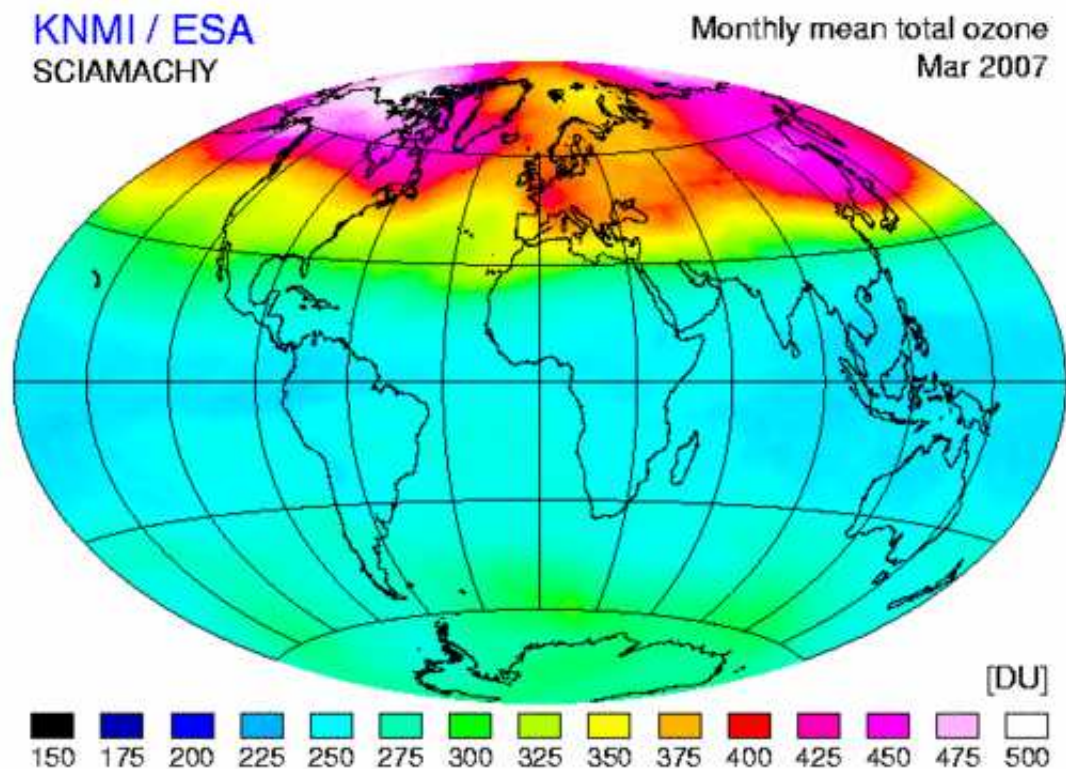
The SO₂ peak values shown in the image satisfy the [criteria for exceptional SO₂ concentration](#) and would thus trigger an alert, but clearly this is a "false alert". In fact, the plot shown here comes from the dedicated web page that shows this alert.

Apparent band of higher SO₂ at mid-latitudes



The monthly average SO₂ slant column plots show in most cases a kind of band of higher and noisier SO₂ signal between about 30 and 60 degrees North. See for example the plot for March 2007 shown here, which shows a particularly clear band. A few months show no or a very weak band at the same latitude. A similar band exists on the Southern hemisphere, but there it is much less pronounced. All in all the SO₂ slant column lies for low and mid latitudes mostly between +0.3 and -0.3 DU, which can be considered as the noise level on the zero-SO₂ background.

Note from the plot shown here that the South Atlantic Anomaly is clearly visible as enhanced noise in the SO₂ slant column.



It is unclear what the origin (reason) for this band is. Most likely it has to do with not entirely adequate correction of the ozone interference. But it is strange that the band lies at slightly lower latitudes than where the largest variation of ozone along latitudes is observed, as can be seen by comparing the monthly average total ozone column with the SO₂ plot above.

Reference spectra -- *SCIAMACHY* data

The slant column retrieval algorithm requires a reference spectrum without the presence of absorption features of the trace gas to be retrieved, since the DOAS method is based on the difference in absorption between two spectra. The reference spectrum can in principle be a solar spectrum, but since the solar spectra from SCIAMACHY showed problems in the past, an earthshine spectrum is used as reference spectrum.

For the SO₂ slant column retrieval a reference spectrum without any SO₂ absorption must therefore be selected. A good geographic region to do this is around the equator above the Pacific or Indian ocean, as there are no sources of SO₂ located there. As instrument characteristics may vary over time, it is necessary to regularly update the reference spectrum with time.

For the retrieval for the Volcanic & Air Quality SO₂ Services, a new reference spectrum is selected in principle once every month at around the middle of the month, depending on availability of the data, from a measurement south-west of the southern tip of India, at about 65 degrees East and just south of the equator.

Since the reference spectrum changes every month, the correction for the offset in the SO₂ background level is determined for each month separately.

Archive services

In the off-line processing of a given month for the Archive Services, the reference spectrum and the offset correction are determined from the data of that month.

Near-real time services

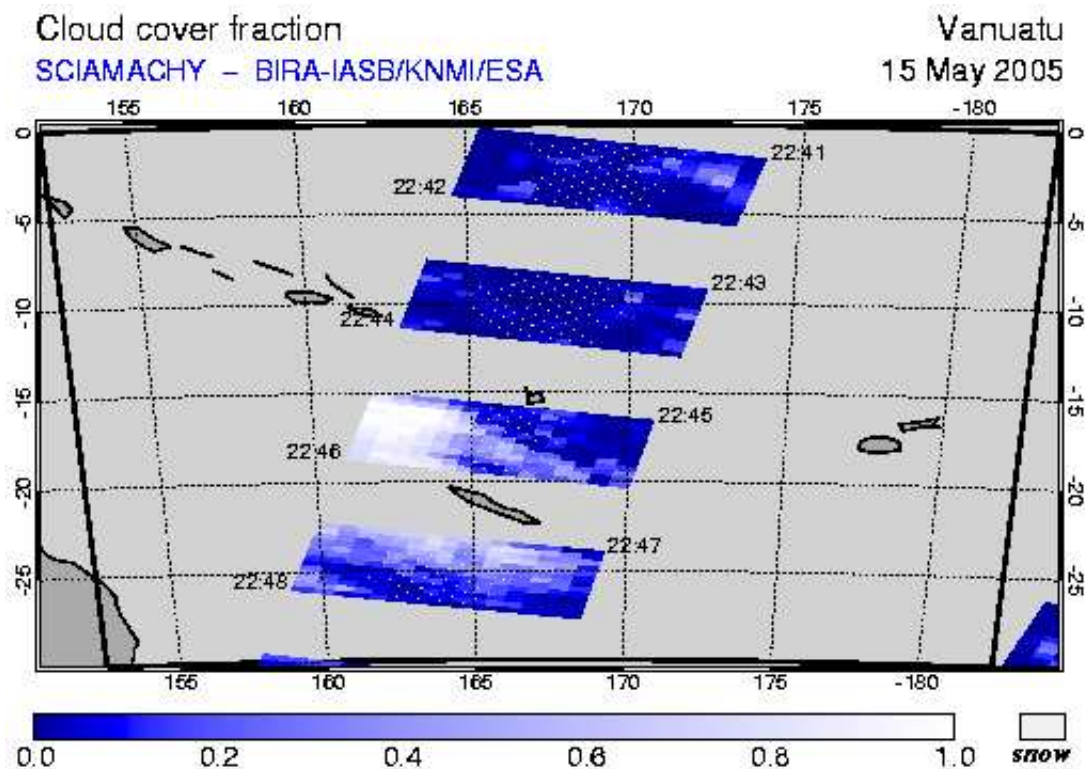
For the near-real time SO₂ processing, selecting a reference spectrum from the current month is not possible, as determining the background offset correction requires all data of a full month. For that reason the NRT service uses the reference spectrum from the most recent month for which the offset has been determined.

At some point in time, when all data of the month is available, the month is reprocessed for the Archive Service, using an appropriate reference spectrum and background offset correction.

Cloud cover fraction

As additional service to interpret the SO₂ (vertical and slant) column densities, the web pages that show images of the SO₂ data also show an image of the cloud cover fraction for the same region, taken from the same instrument. Note that currently there is *no* cloud screening performed on the data: all SO₂ slant column retrieval results are shown as-is.

The same cloud fraction is also used to determine the air-mass factor (AMF) when taking the AMF from look-up tables made with a radiative transfer model in order to compute the SO₂ vertical column density. Note that the AMF and thus the vertical column cannot be calculated if the cloud cover fraction is missing.



For the daily data at orbit (*like the image shown here*) and at grid coordinates, as well as for the 3-day composites at grid coordinates [GOME-1 and SCIAMACHY only], the cloud cover fraction is presented in the same way and available in the accompanying data files. Monthly averages of the cloud fraction are not made: there is no cloud screening method applied to the SO₂ data, so that a monthly average cloud fraction does not provide any useful additional information.

The cloud fraction is a number between zero (clear-sky: no clouds) and one (fully clouded, also known as overcast). For the Volcanic & Air Quality SO₂ Services the cloud data is taken from existing data products:

- For SCIAMACHY data, the cloud fraction is taken from the data files generated by the FRESKO algorithm, which derives the cloud data from the Oxygen A-band (between 758-775 nm). See [this page](http://www.temis.nl/fresco/) (<http://www.temis.nl/fresco/>) at the TEMIS website for more information and data.

The FRESCO cloud data is either in "normal mode" or in "snow/ice mode". In the latter case, a cloud fraction of one is assumed with the cloud at ground level when determining the AMF for the SO₂ vertical column. In the datafiles, however, the cloud fraction in the "snow/ice mode" is set to '-1', and it is shown in a separate colour in the cloud fraction images (indicated simply as "snow" in the colour bar).

Note that the FRESCO cloud cover data retrieval strictly speaking is based on sunlight reflected by a combination of clouds and (reflecting) aerosols: such aerosols are effectively treated as clouds. This means that the FRESCO data product contains a (small) aerosol contribution.

- For GOME-1 data the FRESCO cloud product is also used; for some details see the SCIAMACHY description above.
- For OMI data, the cloud fraction is taken from the level-2 data product provided by NASA/NOAA.

The "quality flags" of the ground pixel in that data product gives the presence of snow or ice. The following situations are taken to represent the "snow/ice mode": permanent ice, dry snow, and a sea ice concentration of more than 50% -- all other cases are considered to be "normal mode"

- For GOME-2 data ... [*to be added*]

Near-real time SO₂ data service

On 27 September 2006 the near-real time (NRT) processing of SO₂ slant column data based on SCIAMACHY observations for both the Volcanic & Air Quality Services was made available. Maps based on OMI data are presented in NRT since 8 November 2007. Links to the data sets are given above[at the website]. The term "near-real time" usually means: within 3 to 6 hours after observation.

Based on the SCIAMACHY data, the system also sends notifications (or: alerts) of exceptional SO₂ concentrations by email to users who have subscribed to that service; see [this page](#)[at the website] for an introduction and description of what is provided by the alert service.

This NRT service provides data and images to the website. For this service, only data files and images with the data on satellite orbit coordinates are provided. The software processes incoming SCIAMACHY level-1 files in NRT. On a given day, the processing will involve only measurements of that day and the day before: processing older data is not very useful for the notification system.

By far most SCIAMACHY orbits are processed within about 5 hours after observation. But a few orbit from the beginning of the day (in terms of UTC) often arrive later than orbit from the middle or end of that day -- this is due to the late delivery of the data by the ground data network.

Images in the near-real time service

The data services based on SCIAMACHY data provide images of the SO₂ slant columns (SCD) and vertical columns (VCD) and of the cloud cover fraction (CCF). In order to convert the SCD into the VCD, information on the clouds is necessary: if the CCF is not available, the VCD cannot be computed. In the archive service one will thus see no VCD where there is no CCF.

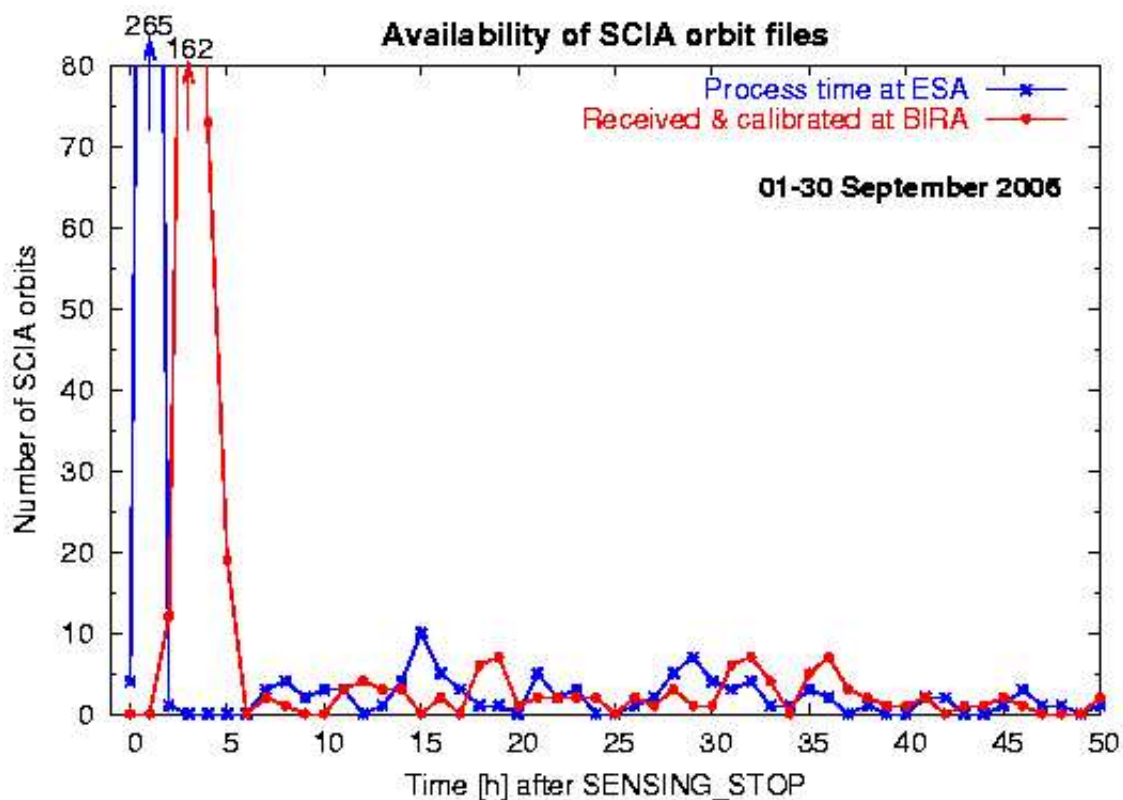
In the NRT service, things are a little different. Since the main goal of the NRT service is to give information on the location of SO₂ peak values possibly related to volcanic eruptions or anthropogenic activities, it is not necessary that the values are exact. To at least have an idea of where SO₂ peaks are related and a rough estimate of the total column of SO₂ in the absence of cloud information, the VCD is calculated assuming clear-sky conditions, i.e. the absence of any clouds.

For OMI data there is no real SCD available, as the SO₂ concentration is derived in a different way. Therefore only images of the VCD and CCF are available.

Process monitoring

Processing of SCIAMACHY data is currently done at BIRA-IASB. The service is run on a best-effort basis, without much process monitoring, as the service is still in an experimental stage. The graph below gives an indication of the time between the measurement and the availability of the data.

Processing of OMI data is done by NASA/NOAA and the level-2 data is delivered in NRT to KNMI, where the plotting is done in NRT.



Graph showing how many SCIAMACHY orbit files are available as function of the hours after the end of the measurements along that orbit. The blue curve gives the time it took ESA to process the raw data and prepare the level-1b spectrum files. Once these files are made, they are made available to, among others, KNMI. From KNMI they are pushed to BIRA-IASB, where they are picked up and calibrated (to form level-1c files) for the retrieval of trace gases, such as NO₂, SO₂ and BrO. The red curve shows the time to took for that step to be finished.

Criteria for exceptional SO₂ concentrations

The near-real-time processing issues a notification (or: alert) of exceptional SO₂ concentrations by email to users who have subscribed to that service; see [this page](#)[at the website] for an introduction and description of what is provided by the alert service.

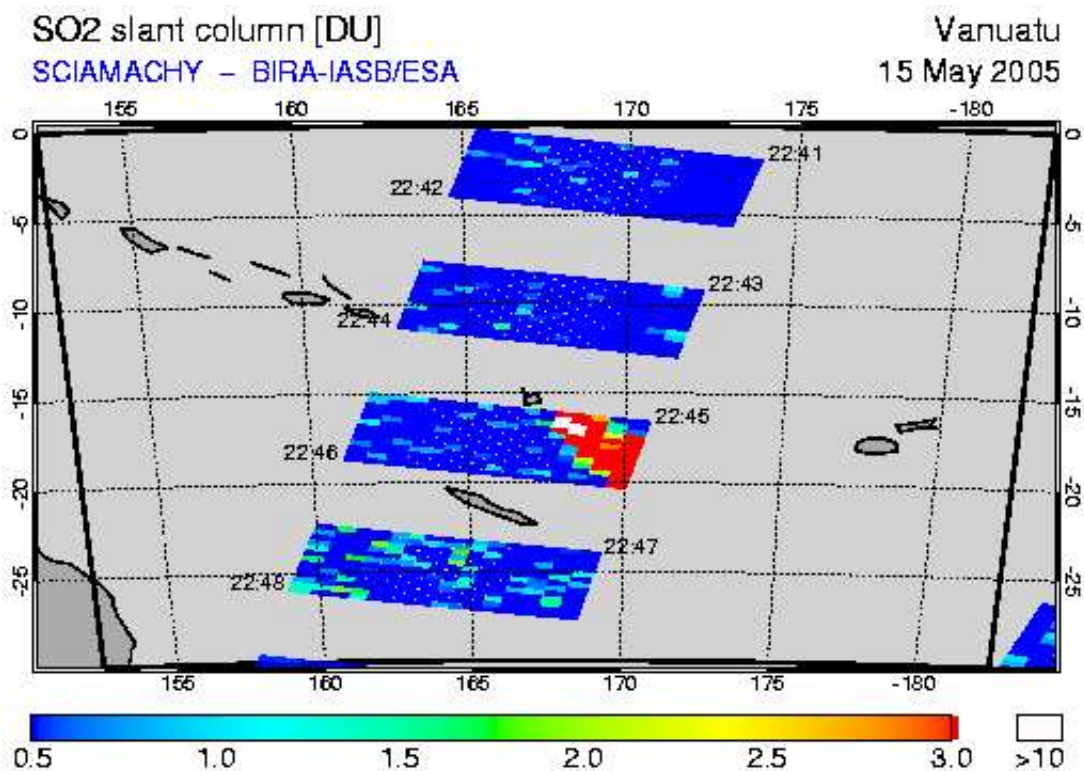
The criteria for exceptional SO₂ concentrations for the SO₂ data have been set up by examining the results of the retrieval and analysis processes. The results of alert events found by the processing are the source for the continuous (qualitative) validation of the alert service.

Since the measurement method and data structure of different satellite instruments is different, the criteria for an alert necessarily have to be different too.

Though the GOME-1 instrument is still operational, it has limited coverage due to permanent failure of some satellite systems, which makes it unsuitable for use in an NRT alert service. Therefore no selection criteria are set up for GOME-1 data.

Criteria for SCIAMACHY data

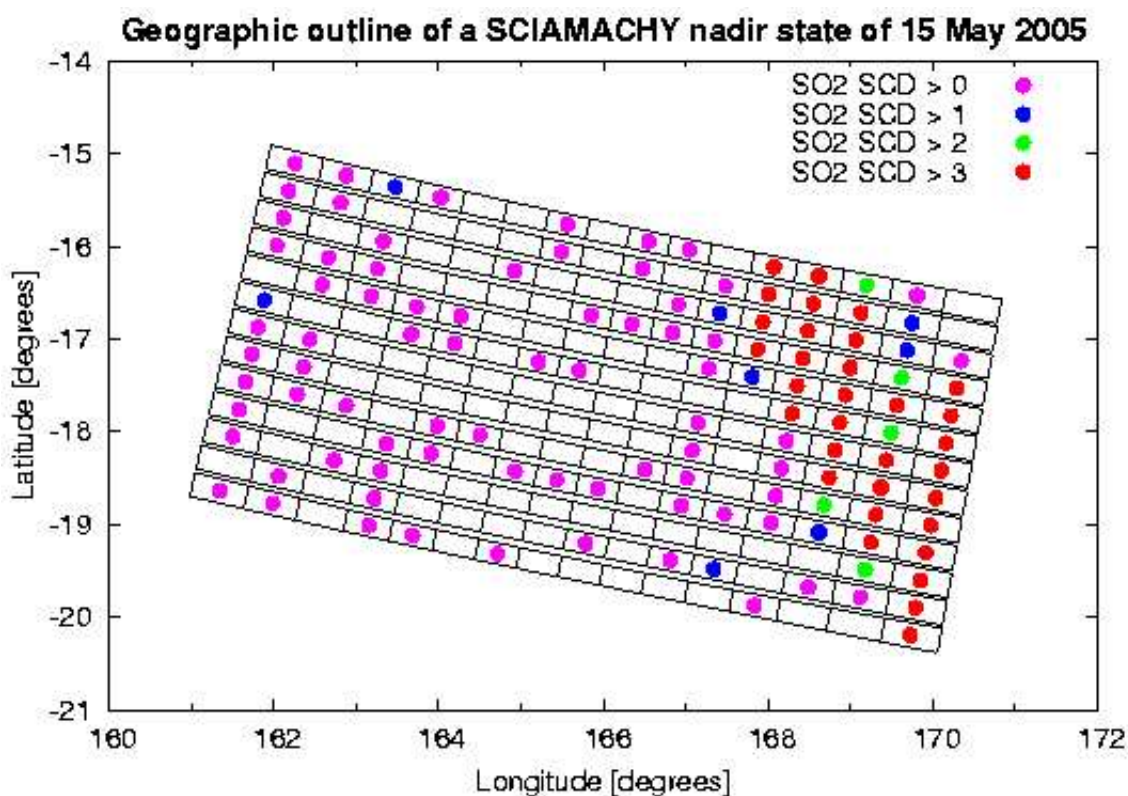
SCIAMACHY measurements alternate between a nadir and a limb viewing mode. For the SO₂ retrieval only the data of the nadir viewing mode can be used, hence the gaps in the plots of the orbits. With this manner of measuring in mind, the natural entity of SCIAMACHY data is a nadir state, which consists of 13 forward and backward scans of 960 km wide (in the normal viewing modes). In the forward direction a nadir state measures about 500 km.



For the analysis only the ground pixels part of each forward scan are considered; these are also the pixels plotted in daily data at orbit coordinates, an example of which is given in this graph of the SO₂ slant column.

Since the vertical column density (VCD) depends on quite a few assumptions and is only available when cloud cover information is available, the VCD is not a suitable quantity to use for setting up selection criteria for alerts. Instead the slant column density (SCD) is used, after the background correction has been applied.

The following graph shows an geographic overview of all the forward ground pixels of the nadir state just below the centre of the above SO₂ slant column plot. A coloured circle in each ground pixels indicates the value of the SO₂ slant column. Note that if the SO₂ concentration is very low, then the DOAS retrieval may results in a negative slant column, with an error that is of the same magnitude.



Geographic outline of the SCIAMACHY nadir state just below the centre in the first graph. The blank rectangles show the outlines of the forward pixels of the nadir state. Colour circles indicate the level of the SO₂ slant column (SCD); empty ground pixels have a negative SCD, which indicates that there is very little to no SO₂.

On the basis of this schematic outline the following procedure is followed to see whether the nadir state should trigger an alert to be issued. For each ground pixel in the nadir state that has an SCD of more than 3 DU, the pixels around it are scanned. Each of these eight pixels that have an SCD greater than 3 DU counts as +1 point. And each of these pixels that have an SCD less than zero counts as -1 point, as sharp gradients in the SO₂ (i.e. from +3 to less than zero) usually indicate that the signal may not be real.

The maximum number of points awarded to any given ground pixel in the nadir state is thus 8. If the number of points is 5 or more, then an alert is issued for this nadir state.

For ground pixels along the edges of a nadir state things are a little different as part of the information needed is missing: it lies outside the state. For that reason, the two points one further along the edge are also considered in the awarding of points, while one point is subtracted because the pixel is at the edge. This means that ground pixels along an edge of the state can be awarded at maximum 6 points and can therefore also trigger an alert. (For ground pixels in the corners there really is too little information available to let these trigger an alert.)

To see which predefined geographic regions are to mentioned in the alert for the current state, it is checked within which of these regions lie the centre coordinates of the individual ground pixels of the nadir state. For a geographic region to be marked the centre coordinate should lie inside the region by at least 2 degrees in latitude and longitude.

Criteria for OMI data

[To be defined]

Criteria for GOME-2 data

[To be defined]

Air-Mass Factor using Look-up Tables

There are two approaches taken to convert the SO₂ slant column density (SCD), retrieved with a DOAS technique, into a vertical column density (VCD). Both approaches use an air-mass factor (AMF). This page describes the determination of the air-mass factor using pre-calculated look-up tables, made with an off-line radiative transfer model.

The approach described here is applied to data from GOME-1, SCIAMACHY and GOME-2, with only minor differences necessary to take the differences between the instruments (such as the viewing geometry) into account. For OMI data the approach is rather similar, though there is no real SCD available; for info and links see the section on the [SO₂ column from OMI](#).

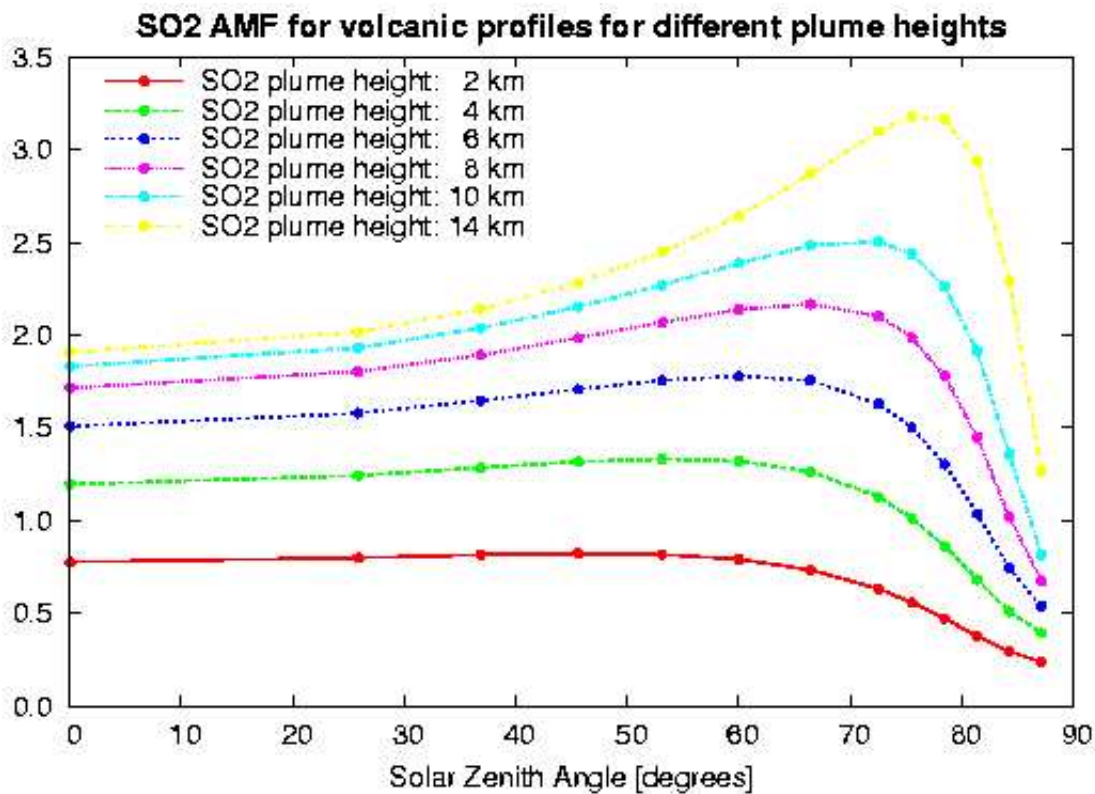
Determining the air-mass factor

The value of the AMF depends on the length of the light path, the vertical distribution of absorbing trace gas in the atmosphere, the reflectivity (albedo) of the earth's surface, etc. The length of the light path depends on the position of the Sun (expressed in the Solar Zenith Angle, SZA) and the angle under which the satellite is looking at the atmosphere. For the vertical distribution a-priori information on the SO₂ profile is used, based on realistic concentrations.

If there are clouds in the atmosphere, things become more complicated. Clouds namely reflect (and scatter) incoming sunlight and thus effectively shield all that is going on below the clouds from the satellite's view. Clearly, the satellite measurements provide an SCD which contains only information on the atmosphere *above* the clouds. To treat this situation, an "effective" AMF is computed, taking the cloud fraction (which gives the percentage of the cloud cover) into account. In the presence of clouds the VCD is clearly less accurate than the VCD derived under clear-sky conditions.

The AMF is pre-calculated with the radiative transfer model LIDORT in the form of a look-up table with a set of entries: the time of the year, the viewing geometry, the SZA, the surface albedo, the cloud fraction and cloud top pressure, etc. Depending on the value of the SCD of SO₂ (low or high), a likely a-priori SO₂ profile is chosen and an AMF is interpolated from the look-up table. The look-up table does not have an entry for the ozone concentration, as the SO₂ AMF depends only weakly on the ozone concentration; an ozone concentration of 350 DU was assumed for the look-up table.

In order to find the AMF the elevation of the SO₂ plume (or: cloud) must be given, as the AMF is different for different SO₂ plume heights. This is shown in the following image for a typical viewing geometry. The look-up table therefore also has an entry for the plume height; for the look-up table it was assumed that the thickness of the plume is 1 km (this value is not very critical).



Air-mass factors (AMF) as function of Solar Zenith Angle (SZA) for an SO₂ plume of 1 km thickness and with low to moderate SO₂ concentrations (up to 10 DU). The viewing geometry is looking straight down to a surface with albedo 0.05 at about sea-level.

In the practice of the SO₂ retrieval, especially in an automatic processing, there is no information available on the altitude of the SO₂ cloud. But the latter is not known from the retrieval in an automated processing, so an assumption must be made. It has been decided that the VCD is computed for three different assumed plume heights, with in all cases an assumed plume thickness of 1 km:

- 1 km above local ground level
- 6 km [or 1 km above local ground level, if that is higher]
- 14 km

The first one represents passive degassing of volcanoes and anthropogenic activities, the second one moderate volcanic eruptions and the third one explosive eruptions. These numbers agree more or less with what is done for the SO₂ column derived from OMI data.

All three VCDs based on these assumptions are available in the data files, whereas the middle one is used for the plots presented on these web pages. To find an estimate of the VCD for another plume height, one could linearly interpolated between the three given values. The SCD is also plotted and can be accessed under "other plots".

If the VCD is available, images of it are shown on the website and the values are given in the data files. The data files also given an error estimate, which simply is the SCD error estimate divided by the AMF; possible errors in the AMF calculation are therefore not taken into account.

If no cloud cover information is available for a given ground pixel, the AMF and VCD of that ground pixel cannot be computed. In that case, the entries in the data files will get the "no data" value. Only the AMF for the clear-sky part will be given a value, as that can in principle be computed always.

Air Mass Factor using a Chemistry Transport Model

There are two approaches taken to convert the SO₂ slant column density, retrieved with a DOAS technique, into a vertical column density. Both approaches use an Air-Mass Factor (AMF). This page describes the use of a chemistry transport model to obtain this air mass factor.

In this approach the retrieval of the VCD for SO₂ will be based on a combined retrieval/modelling approach, similar to the approach for some other trace gases (such as formaldehyde, HCHO). The main motivation for this new approach is to improve the accuracy of the retrieval. A chemistry-transport model (TM4), driven by high-quality meteorological fields from ECMWF, will provide best-guess profiles of SO₂, based on the latest emission inventories, atmospheric transport, photochemistry and wet/dry removal processes.

These model forecast fields will be collocated with the satellite (GOME, SCIAMACHY, OMI) observations, and the radiative transfer modelling in the retrieval will be performed based on the model trace gas profile and temperature profiles. The retrieval is coupled to cloud top height and cloud fraction retrievals derived from the satellite data, and the retrieval will be coupled to high quality albedo maps.

NOTE

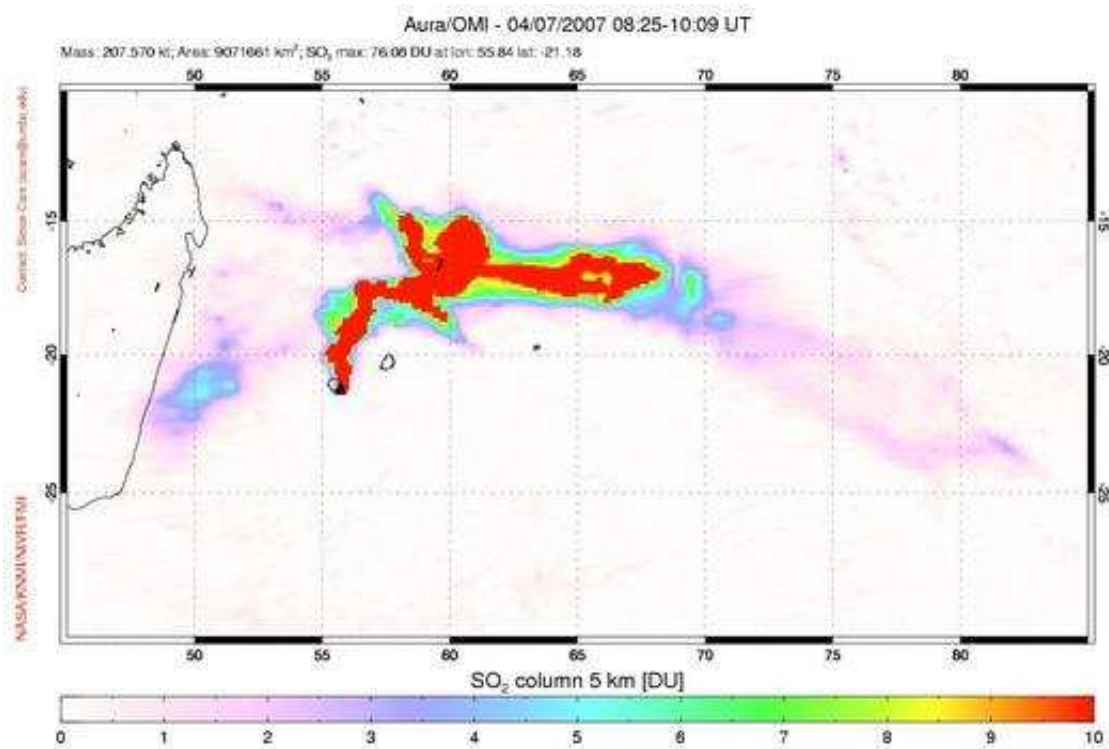
*This approach is currently not under evaluation.
Possibly it will be picked up again at a later stage.*

SO₂ total column based on OMI data

The SO₂ data product based on observations of the GOME-1, SCIAMACHY and GOME-2 instruments are determined using a DOAS algorithm to determine the slant column density followed by the use of an AMF pre-determined with a radiative transfer model to find the vertical (total) column density.

The SO₂ data product based on OMI data is derived quite differently -- namely with a "band residual method" using the residuals of the DOAS-based ozone retrieval -- and it does not give a comparable slant column density as intermediate step. The method used for OMI should in principle lead to the same SO₂ total column as those derived with the other methods.

The OMI data product file contains three estimates of the total SO₂ column in Dobson Units. These correspond to three a-priori vertical profiles for the SO₂ vertical distribution used in the retrieval algorithm. The three vertical profiles were selected to represent typical SO₂ vertical distributions for three SO₂ source regimes: SO₂ in the Planetary Boundary Layer (PBL, below 2 km) from anthropogenic sources, SO₂ distributed between 5 and 10 km emitted by passive volcanic degassing in the free troposphere, and SO₂ distributed between 15 and 20 km representing injection from explosive volcanic eruptions. The images shown on the website represent the second of these three regimes.



SO₂ total column based on OMI measurements on 7 April 2007. The SO₂ plume is related to the eruption of the Piton de la Fournaise volcano on Reunion Island, which started a few days earlier and continued for several days. [Image courtesy Simon Carn, OMI/NASA.]

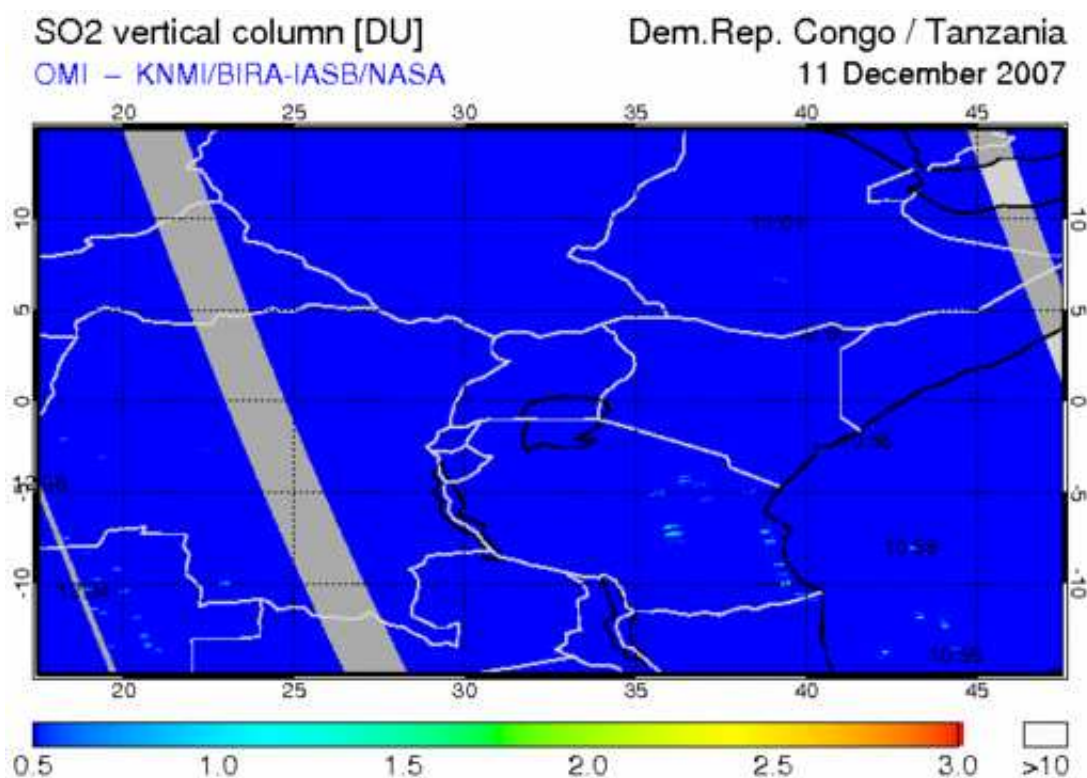
In the OMSO₂ product, all PBL data are processed with the Band Residual Difference (BRD) method, while all 5 km and 15 km data are processed with the Linear Fit (LF) algorithm. The algorithms use different subsets of calibrated residuals produced by the NASA operational ozone algorithm. This set contains residuals centered at the Earth Probe (EP) TOMS wavelengths, four residuals at extrema of

the SO₂ absorption cross-section from 310.8-314.4 nm, and two non-absorbing wavelengths at 345 and 370 nm. Both OMSO₂ algorithms use the temperature-dependent SO₂ cross-sections data, residual correction for background regions, and different parameterizations of the AMF.

The BRD algorithm uses differential residuals at 3 SO₂ sensitive OMI UV2 wavelength pairs, and the pair average is used to produce all PBL data. A constant AMF of 0.36 is used to estimate total SO₂ (vertical column). For strong volcanic degassing and eruptions, SO₂ loading can be very large and the BRD algorithm may fail. The LF algorithm has been developed to optimally select residuals from the set of available OMTO3 bands to retrieve SO₂ under these conditions. The LF algorithm minimizes a subset of the residuals by simultaneously adjusting total SO₂, total column ozone, reflectivity at 331 nm, and polynomial coefficients (linear and quadratic) to account for the wavelength dependent effect of surface albedo and aerosol on the effective reflectivity.

More information, references and links regarding the OMI SO₂ data product can be found at the website of the [Aura OMI Sulphur Dioxide Data Product](http://disc.gsfc.nasa.gov/Aura/OMI/omso2.shtml) (<http://disc.gsfc.nasa.gov/Aura/OMI/omso2.shtml>) See also the website of the [OMI Sulphur Dioxide Group](http://so2.umbc.edu/omi/) (<http://so2.umbc.edu/omi/>)

OMI SO₂ data presented on this web site



This website contains maps (plots) of the SO₂ distribution based on OMI measurements. The maps presented here use exactly the same colour bar as is used for data of other satellites, so that it is easy to compare the results.

The image here shows the SO₂ distribution (in this case there is virtually no SO₂) over Dem.Rep. Congo. The times of the measurement are plotted at the middle of each orbit, once every 50 swaths. The image also shows bands of no data: pixels 53 and 54 of the swath -- these have an instrumental problem and since that can lead to a spurious SO₂ signal, the pixels are omitted from the OMI plots.

Note that in the NRT service only images are shown; data files are not supplied. The archive service provides images and links to data files.

Time period of the data in the SO₂ archive

Data for the Air Quality and the Volcanic SO₂ Archive & Near-real time Services have been / are computed for the following time periods:

<i>instrument (satellite)</i>	<i>time period of data</i>	
	<i>Archive service</i>	<i>NRT service</i>
GOME (ERS-2)	[to come]	[not applicalbe]
SCIAMACHY (ENVISAT)	September 2004 -- December 2007	01 August 2007 -- present
OMI (EOS-Aura)	[to come]	24 October 2007 -- present
GOME-2 (MetOp-A)	[to come]	[to come]

Missing data in the SO₂ data archive

The satellites carrying the instruments perform 14 or 15 orbits per day. It happens that for one or more of these orbits data is missing, either because the instrument did not measure anything, or because the measurement is of too low quality for a reliable retrieval. This missing data leads to gaps in the plots of the daily data. For some geographic regions of either of the two Services the web pages accessing the data archive will then show empty pictures.

There are also days with no data at all, again because of lack of measurements or lack of the quality of these measurements. For these days there will be no data in the archive at all, and the web pages accessing the data archive will show a message.

The following tables lists full(!) days without any data; these table is maintained by hand and may thus be incomplete.

SCIAMACHY

Year	Month	Days
2008		
2007	December September	02-04 25-27
2006	December November September April	13-15 29 08-10 06-08, 17-19
2005	May January	12 01-02
2004	December November October September	20-31 17 01 23

OMI -- *to check*

Year	Month	Days
2008		
2007		

GOME-2 -- *to check*

Year	Month	Days
2008		
2007		

Specification of the data file formats

The data used to make the images (maps) available at the website are in general also available in some form. Both the availability and the form depend on the satellite instrument:

- [SCIAMACHY based data](#)
- [OMI based data](#)
- GOME-1 based data -- *not available yet*
- GOME-2 based data -- *not available yet*

See also the section on the [Presentation and delivery of the data](#). Links to the relevant data files -- if available -- are given on the web pages showing the images (maps).

SCIAMACHY based data

The SO₂ data based on SCIAMACHY is delivered in two forms:

- as ASCII files for daily data at the coordinates of the measurements, in other words: at orbit coordinates
- as HDF-4 files for daily data, 3-day composites [SCIAMACHY and GOME-1 only] and monthly averages at the coordinates of a rectangular latitude-longitude grid

The data product files mention, among others, version number (see the chapter [Process version history](#)). They also have been given a *product status*, for a quick-look indication on the status of the data product:

<i>status</i>	<i>description</i>
NRT data	for SO ₂ column data delivered via the Near-real time Service (only for the ASCII data files)
preliminary data	for data delivered via the Archive Service, either just the slant column, or including a preliminary vertical column
archive data	for slant column and vertical column data delivered via the Archive Service

The data file structure is described on separate pages:

- [ASCII data format specification](#)
examples:
 - [Reading and plotting an ASCII data file with IDL](#)
 - [Reading and plotting an ASCII data file with Fortran](#)
- [HDF data format specification](#)
examples:
 - [Reading and plotting an HDF data file with IDL](#)

====> Some notes regarding downloading of data files and images

OMI based data

The SO₂ data based on OMI measurements at orbit coordinates is provided by NASA in their HDF5-EOS format. The NRT data used for the images is not available for download to third parties. The off-line data usually follows 2 or 3 days later and is available via the NASA website via [this page](http://disc.gsfc.nasa.gov/Aura/OMI/omso2.shtml) (<http://disc.gsfc.nasa.gov/Aura/OMI/omso2.shtml>), which also gives access to a description of the (rather complex) data format.

It is not yet certain whether daily composites of OMI data on a latitude-longitude grid will be made. Monthly average data will be provided on the same grid as the SCIAMACHY data, in the same format: HDF-4; see the links above for more information.

Specification of the ASCII data file format

-- *SCIAMACHY data*

The daily data at coordinates of the measurements by the satellite instrument are delivered in the form of ASCII files, one for each orbit file with spectral data. Measurements of SCIAMACHY come in principle as one file per orbit, but it happens quite often that files span only a part of an orbit, or even the end of one orbit and the beginning of the next. The data files are delivered via the website as zip-files containing all orbit files of a given day.

See the main [Data format specification page](#) for some general notes on the data formats.

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 start time HHMMSS, both taken from the name of the original measurement file:

```
so2cdYYYYMMDD_HHMMSS.dat
```

where so2cd stands for "SO2 column density". These files contain the SO2 slant column data (SCD) and -- if available -- the SO2 vertical column density (VCD) derived with an appropriate air-mass factor, and the cloud cover fraction.

The ASCII data file can be read easily with, for example, a Fortran program ([example page](#)) for further processing. The ASCII file can also be read with many plot programs, such as IDL ([example page](#)) and MatLab.

File header

Each data file has a header with comment lines (starting with the # mark), giving orbit and analysis information, as well as a list of the data columns. Also given is for format of each data fields, and the full data format for reading the data lines. A typical data file header for data files looks as follows. Some remarks regarding the entries in the file header are given [below the file header](#).

```
# SO2 column density for TEMIS / PROMOTE
# -----
#
# Product status   : archive data
# Process version : 1.0.3
#
# Instrument       : SCIAMACHY
# Orbit date/time  : 20070320_120511
# Orbit number     : 26416
#
# Analysis date    : 2007/08/13
# Cloud cover data : FRESCO (SC-v5)
# AMF & VCD values: yes
#
# Nr plume heights: 3
# Nr data columns : 47
#
# Data columns                                           [format]
#
```

```

# --- Ground pixel data
#   1 = measurement date as YYYYMMDD           [a8]
#   2 = measurement time as HHMMSS.SSS         [1x,a10]
#   3 = pixel id: 0=forward, 3=backscan         [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 correction
#   18 = retrieval error on the SCD (in DU)      [f9.3]
#   19 = chi^2 of the slant column fit (x 1e-6)  [f9.3]
#   20 = slant column value index (SVI)         [i4]
#         0 : SO2 SCD <= 1.5 DU
#         1 : SO2 SCD > 1.5 DU, no alert issued
#         2 : SO2 SCD > 1.5 DU, alert issued for state
#
# --- Vertical column data
#   21 = AMF quality index (AQI)                [i4]
#         = -1 : no AMF calculation selected
#         = 0 : successful AMF calculation
#         = +1 : no cloud cover data available
#         > +1 : error computing AMF
#   22 = AMF profile shape number (1 or 2)      [i4]
#         --- using plume height #1 = 1.0 km above surface
#   23 = SO2 vertical column density VCD (in DU) [f9.3]
#   24 = Error on VCD from column 18 (in DU)    [f9.3]
#   25 = Total air-mass factor (AMFtot)         [f9.3]
#   26 = AMF for clear-sky part (AMFclr)        [f9.3]
#   27 = AMF for cloudy part (AMFcld)          [f9.3]
#         --- using plume height #2 = 6.0 km *
#   28 = SO2 vertical column density VCD (in DU) [f9.3]
#   29 = Error on VCD from column 18 (in DU)    [f9.3]
#   30 = Total air-mass factor (AMFtot)         [f9.3]
#   31 = AMF for clear-sky part (AMFclr)        [f9.3]
#   32 = AMF for cloudy part (AMFcld)          [f9.3]
#         --- using plume height #3 = 14.0 km *
#   33 = SO2 vertical column density VCD (in DU) [f9.3]
#   34 = Error on VCD from column 18 (in DU)    [f9.3]
#   35 = Total air-mass factor (AMFtot)         [f9.3]
#   36 = AMF for clear-sky part (AMFclr)        [f9.3]
#   37 = AMF for cloudy part (AMFcld)          [f9.3]
#         *) or 1 km above surface if that is higher
#
# --- Cloud and Surface data
#   38 = cloud cover index (CCI)                [i4]
#         = 0 : no cloud cover data
#         = 1 : clear sky mode
#         = 2 : normal FRESCO mode
#         = 3 : snow/ice FRESCO mode
#         = 4 : missing or invalid FRESCO data

```

```

#      39 = cloud fraction                                [f9.3]
#      40 = cloud top pressure (in hPa)                  [f9.3]
#      41 = cloud top height (in km)                    [f9.3]
#      42 = cloud top albedo                             [f9.3]
#      43 = surface pressure (in hPa)                   [f9.3]
#      44 = surface elevation (in km)                   [f9.3]
#      45 = surface albedo                              [f9.3]
#
# --- Additional ground pixel data
#      46 = sciamachy state_index                        [i4]
#      47 = sciamachy state_id                          [i4]
#
#
# Full data format: (a8,1x,a10,i4,16f9.3,3i4,15f9.3,i4,7f9.3,2i4)
#
#

```

Which is followed by two lines spanning all 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.

```

The first part of the comments gives some general information on the orbit and retrieval. The number of data columns in the file depends on the number of plume heights used for computing the AMF and VCD, hence both these numbers are given here. The first 22 columns are always present. Then follow sets times five lines, one set for each plume height. And the last 9 columns are always present.

If no vertical column densities (VCDs) have been computed, then:

- the `AMF & VCD values` comment line in this part of the file says `no` ;
- the AMF quality index (AQI) in column 21 is set to -1;
- all data entries concerning the AMF and VCD are given the "no data" value (-99.0), except where possible the clear-sky AMF (see below).

If cloud cover information is included, as in the example, the source of the cloud data is mentioned. If no cloud cover information has been included, then:

- the `Cloud cover data` comment line in this part of the file says `none` ;
- the cloud cover index (CCI) in column 38 in the above example is set to 0;
- all data entries concerning the cloud cover, the AMF and VCD are given the "no data" value (-99.0).

and no AMFs or VCDs can be computed.

Remarks

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 (0) and backward (3) scan pixels.
- 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 error value given in column 18 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 19 is also a measure of the quality of the fit. In fact, these three quantities are all interlinked: $\text{chi-square} = \text{RMS} * \text{RMS}$, and the relationship between the slant column error and the RMS is assumed to be linear. To assist data users in their analysis, both the slant column error and the chi-square are written to the data file.
- The "slant column value index" (SVI) in column 20 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 the notifications on exceptional SO₂ concentrations.
- If an AMF and VCD have been computed, the "AMF quality index" (AQI) in column 21 indicates success of the AMF computation, and if successful the VCD was computed. The relevant AQI values are listed in the file header; more details are given on a [separate page](#).
- Column 22 gives the number of the profile used for the AMF computation, which depends on the SO₂ concentration: '1' for low concentrations, '2' for high concentrations; more details are given on the [Air-mass factor using look-up tables](#) info page.
- In order to compute the AMF, a height must be given of the SO₂ plume. As this height is not known automatically, a number of assumed heights are used, in this case three. For each assumed plume height, the data file gives five quantities: the SO₂ vertical column, an estimate of the error on it (based on the error given in column 18), and the three components of the AMF; more details are given on the [Air-mass factor using look-up tables](#) info page.
- If cloud cover data is included, the "cloud cover index (CCI)" in column 38 in the above example indicates success of this inclusion. The relevant CCI values are listed in the file header; some more details are given on a [separate page](#).
- Data fields for which no value was (successfully) computed are given the "no data" value -99.

Data flags in the ASCII data file

The ASCII data files of the SO₂ service contain some flags (see the [ASCII data file specification](#)):

- [AMF quality index \(AQI\)](#)
- [Cloud cover index \(CCI\)](#)

The meaning of the values of these flags is listed below.

AMF quality index (AQI)

The AMF quality index (AQI) flags the determination of

- data needed by the AMF, such as surface height, surface albedo and geometrical AMF
- the actual AMF computation

<i>AQI</i>	<i>description</i>	<i>allowed range</i>
<i>main flags</i>		
-1	no AMF computation wanted ====> only step 'a' mentioned above is performed	--
0	computation of AMF successful	--
<i>initialisation errors</i>		
1	No cloud cover information available ====> no match with FRESCO data found, or insufficient data available (this combines with CCI = 4; see below)	--
2	Error in surface height array indexing	--
3	Error in surface albedo array indexing	--
<i>error computing geometrical AMF</i>		
4	Solar zenith angle out of range ====> should never occur, as the analysis limits the pixels to SZA <= 85 deg	0. <= solZen < 88.
5	Viewing zenith angle out of range ====> it is unlikely that this will occur	abs(viewZen) < 40.
<i>error computing cloud radiance weight</i>		
6	Error in wavelength	300. <= wavelNm <= 3000.
7	Error in surface pressure	200. <= pSfc <= 1500.
8	Error in cloud-top pressure	10. <= pCld <= 1500.

9	Error in surface albedo	0. <= aSfc <= 1.
10	Error in cloud albedo	0. <= aSfc <= 1.
11	Error in $\mu_0 = \cos(\text{solZen})$	0. <= μ_0 <= 1.
12	Error in $\mu = \cos(\text{abs}(\text{viewZen}))$	0. <= μ <= 1.
13	Error in relative azimuth angle	0. <= dphi <= 180.
14	Error in cloud fraction	0. <= c <= 1.
15	Error in loop over pressure	--
16	Error in radiance weight	0. <= radWeight <= 1.
<i>error computing clear-sky and cloudy SO₂ AMF</i>		
17	Error in interpolation for clear-sky AMF	--
18	Error in interpolation for cloudy AMF	--
<p>Notes:</p> <ul style="list-style-type: none"> Flags 2, 3 and 6 - 16 should in principle not occur; if any of these does occur, something is wrong in the code. Flags 17 and 18 indicate that one of the input parameters of the look-up tables is out of its allowed range. Flags 6 - 18 cannot occur if no AMF computation is wanted (i.e. if only step 'a' is performed). 		

Cloud cover index (CCI)

This flags the cloud cover data used.

<i>CCI</i>	<i>description</i>
0	no cloud cover data
1	clear sky mode ====> the cloud-top pressure set to 1013.0 hPa, the value used internally for the sea-level pressure, and the cloud fraction is set to 0.0
2	normal FRESCO mode
3	snow/ice FRESCO mode ====> for the AMF calculation the cloud fraction is set to +1 and the cloud-top pressure is set to the surface pressure; in the output the cloud fraction is set to -1.0
4	missing or invalid FRESCO data ====> if the AMF is calculated, this combines with AQI = 1 (see above)
With FRESCO v5.1 these flags are adapted to also include sunglint: in case of sunglint "10" is added to the flag; for example flag 11 means "snow/ice + sunglint". Since we are not using sunglint, the flag is simply corrected to be 0,...,4.	

Two adjustments are made to the FRESCO data without any warning or flagging:

- a) If the cloud fraction is < 0.05, the cloud-top pressure is set to 800.0 hPa, as is done in other applications, and the cloud top height to 2.0 km.
- b) The cloud-top pressure P_{ctop} is made to lie in this range:

$$P_{min} \leq P_{ctop} \leq P_{surf}$$
 where the surface pressure P_{surf} depends on the coordinates and the minimum pressure P_{min} is given by the AMF look-up table (which currently is 372.42 hPa).

Reading and plotting an ASCII data file with IDL

The ASCII data files can be read with IDL, for example with the routine [so2ascread.pro](#); this particular routine has been tested at IDL versions 6.0 and 6.3. The routine reads a given number of ASCII files, e.g. all orbits of one day, and plots the SO2 slant column as a simple example.

==> [Return to ASCII data format specification](#)

The files to plot are given in a separate configuration file, the name of which is read by the plotting routine. The structure of the configuration file is given in the header of the [so2ascread.pro](#).

A configuration file listing all orbits of 21 March 2007 [[zip archive of the ASCII data files](#)] [[world plot of the SO2 slant column](#)], for example, looks like this:

```
data/
15
so2cd20070321_011537.dat
so2cd20070321_022800.dat
so2cd20070321_040932.dat
so2cd20070321_055020.dat
so2cd20070321_073247.dat
so2cd20070321_083820.dat
so2cd20070321_101951.dat
so2cd20070321_115931.dat
so2cd20070321_133653.dat
so2cd20070321_151524.dat
so2cd20070321_164850.dat
so2cd20070321_183207.dat
so2cd20070321_200904.dat
so2cd20070321_212242.dat
so2cd20070321_230317.dat
```

When running the example routine with this configuration file, the screen output is:

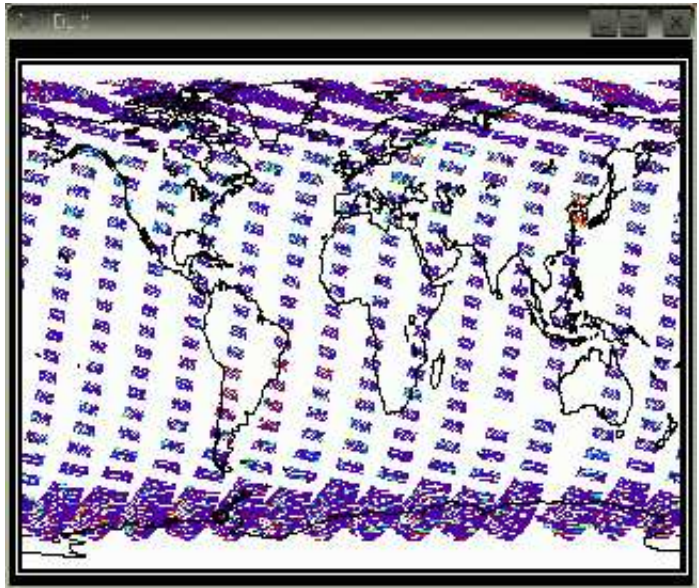
```
IDL> .run so2ascread
IDL> so2ascread

>>> Give the name of configuration file.
: so2ascread.in

--- Reading file so2cd20070321_011537.dat
--- Reading file so2cd20070321_022800.dat
--- Reading file so2cd20070321_040932.dat
--- Reading file so2cd20070321_055020.dat
--- Reading file so2cd20070321_073247.dat
--- Reading file so2cd20070321_083820.dat
--- Reading file so2cd20070321_101951.dat
--- Reading file so2cd20070321_115931.dat
--- Reading file so2cd20070321_133653.dat
--- Reading file so2cd20070321_151524.dat
--- Reading file so2cd20070321_164850.dat
--- Reading file so2cd20070321_183207.dat
--- Reading file so2cd20070321_200904.dat
--- Reading file so2cd20070321_212242.dat
--- Reading file so2cd20070321_230317.dat

IDL>
```

The picture plotted by the routine is shown on the right. It uses a standard IDL colour table and is not ornamented with title, axis labels, etc.; it is merely meant as an example.



Reading and plotting an ASCII data file with FORTRAN

The ASCII data files can be read with FORTRAN for further processing. As mentioned in the [ASCII data format specification](#), the data file has a number of comment lines, which need to be skipped when reading the file.

The Fortran-77 sample program `so2ascread_f77.f` reads the data from a single data file into a set of arrays, and issue a few notes to show that it has read the file.

The header of the sample program specifies how to compile and use it:

```
!
! Compilation:
!
!   FC  -o so2ascread_f77  so2ascread_f77.f
!
! where 'FC' is your favourite Fortran-77 compiler.
! (With '.f' as extention, the file can also be
! compiled with a Fortran-90 compiler.)
!
! Usage:
!
!   so2ascread_f77  SO2datafile
!
! For example:
!
!   so2ascread_f77  so2cd20070321_011537.dat
!
```

Issuing the latter command (prepending the appropriate path to the filename) gives the following output to the screen:

```
--- Reading datafile ...
--- Number of data lines read:      3633
    Date and time of first pixel: 20070321 015449.912
                                last pixel: 20070321 022701.108
```

The actual reading of the data file is done with a subroutine, so that it is easy to make the program read multiple data files.

Reading with Fortran-90 is quite similar, though then it is possible to load the data in one structure, rather than in separate arrays.

Specification of the HDF data file format

Gridded data give the SO₂ concentrations on a rectangular latitude-longitude grid of 0.25 by 0.25 degrees is written to HDF-4 files -- for daily data, for 3-day composites and for monthly averages.

See the main [Data format specification page](#) for some general notes on the data formats.

Simply said, an HDF file has the following structure (note that the vertical column field or cloud cover fraction may not be available):

- File header, with the file attributes
these specify the product name, data, version, units, etc.
- Data sets:
 - SO₂ slant column field
 - Error in the slant column field
from the slant column retrieval
 - SO₂ vertical column field for different plume heights
 - Error in the vertical column fields
from the slant column error
 - Cloud cover fraction

There are several tools around on the web for viewing and treating HDF files, notably at the [NCSA HDF Home Page](http://hdf.ncsa.uiuc.edu/) (<http://hdf.ncsa.uiuc.edu/>). Software for viewing and reading HDF files is available via [this page](http://hdf.ncsa.uiuc.edu/hdf-java-html/) (<http://hdf.ncsa.uiuc.edu/hdf-java-html/>), where you can find a binary distributions for several operating systems (UNIX, Linux, Windows).

The HDF file can also be read with many plot programs, such as IDL ([example page](#)) and MatLab, as well as with the [BEAT toolbox](http://www.science-and-technology.nl/beat/) (<http://www.science-and-technology.nl/beat/>).

Name of the HDF files

The name of the HDF files gives the data (range) of the dates covered by the data sets in the file:

so2cdYYYYMMDD.hdf	file with data for a single day; the name contains the orbit date YYYYMMDD
so2cdYYYYMMDFDL.hdf	file with data for a 3-day composite; the name contains the year, the month and the first (DF) and last (DL) day here: DFDL = 0103, 0406, 0709, , 2527, for February followed by 2828 or 2829, for other months followed by 2830 and 3131 if the month has 31 days
so2cdYYYYMM.hdf	file with data for a monthly average; the name contains the year and month

File header

The following table gives as an example the header of the HDF file of the daily slant column data of 21 March 2007.

<i>Global Attribute</i>	<i>Type</i>	<i>Value</i>
Product	string	SO2 slant column [DU]
Data_version	string	1.0.3
Creation_date	string	26 August 2007
Product_status	string	archive
SO2_field_date_1	integer	2007, 3, 21
SO2_field_date_2	integer	2007, 3, 21
Data_begin	integer	2007, 3, 21, 1, 54, 50
Data_end	integer	2007, 3, 22, 0, 29, 50
Date_format	string	year, month, day, hour, minute, second (UTC)
Instrument	string	SCIAMACHY (ENVISAT)
Cloud_fraction	string	Taken from FRESCO (made by KNMI)
Projects	string	SACS for TEMIS / PROMOTE
Authors	string	Jos van Geffen & Michel Van Roozendaal
Affiliation	string	BIRA-IASB (Belgian Institute for Space Aeronomy)
E-mail	string	josv@aeronomie.be & michelv@aeronomie.be
Number_of_longitudes	integer	1440
Longitude_range	real	-179.875, 179.875
Longitude_step	real	0.25
Number_of_latitudes	integer	720
Latitude_range	real	-89.875, 89.875
Latitude_step	real	0.25
Iscd_field	string	SO2 slant column = Iscd_field/1000 [DU]
Iscd_error	string	Error on SO2 slant column = Iscd_error/1000 [DU]
Number_of_VCD_sets	integer	3
Ivcd_field_#	string	SO2 vertical column (VCD) = Ivcd_field/1000 [DU]
Ivcd_error_#	string	Error on SO2 vert. column = Ivcd_error/1000 [DU]
Iccf_field	string	Cloud cover fraction = Iccf_field/1000 [-]
No_data	string	Entries with -99.0 represent "no data"
Product_code	string	sbfdaa
Data set	Type	Rank --> dimensions
Iscd_field	integer	2 --> 1440 x 720

Iscd_error	integer	2 --> 1440 x 720
Ivcd_field_1	integer	2 --> 1440 x 720
Ivcd_error_1	integer	2 --> 1440 x 720
Ivcd_field_2	integer	2 --> 1440 x 720
Ivcd_error_2	integer	2 --> 1440 x 720
Ivcd_field_3	integer	2 --> 1440 x 720
Ivcd_error_3	integer	2 --> 1440 x 720
Iccf_field	integer	2 --> 1440 x 720

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]".

- **Data_version**

The coding for this is described in the section on the [Data and Services version history](#).

- **Product_status**

This can be "preliminary" or "archive".

- **SO₂_field_date_1 & SO₂_field_date_2**

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 come in principle as one file per orbit. The data included is from all 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.

- **Cloud_fraction**

If no cloud cover fraction is included, the value of this attribute is "None included" and there is no 'ccf' data set.

- **Longitude & latitude ranges and steps**

These are given in degrees.

See [further down](#) on how to (re)construct the longitude-latitude grid of the data sets.

- **Number_of_VCD_sets**

This is the number of different plume heights used to compute vertical column densities (VCDs) and thus gives the number of VCD data sets; which plume heights were used is connected to the version number of the data product.

- **Product_code**

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

- **Data sets**

The above example is for a file which contains the slant column density (SCD), three data sets for the vertical column densities (VCD) and the cloud cover fraction (CCF).

The error values given in the HDF files for the SCD and VCD fields are an average over the error values given in the orbit data files; they include no "standard deviation" of the averaging itself.

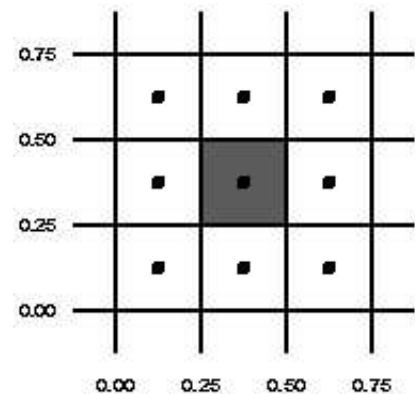
Grid

The data sets in the HDF file are given in the form of a two-dimensional array with each grid cell having a specific longitude-latitude grid. This grid can be (re)constructed using the information given in the header of the HDF file:

$$\text{gridlon}(\text{ilon}) = \text{lonmin} + (\text{ilon} - 1) * \text{dlon}$$

$$\text{gridlat}(\text{ilat}) = \text{latmin} + (\text{ilat} - 1) * \text{dlat}$$

Note that the coordinates of the grid refer to the *centre* of the grid cells, as indicated by the filled circles in the graph on the right.



An example Fortran code for this can be found in the [so2hdfgrid.f](#) program. It generates the grid and gives a few lines of output as example:

```

ilon ilat  gridlon  gridlat
  1    1  -179.8750 -89.8750
1440  720   179.8750  89.8750
  38  562  -170.6250  50.3750
  722  362    0.3750   0.3750
1222   62   125.3750 -74.6250

```

The fourth in this list is the centre of the coloured grid cell in the image.

Reading and plotting an HDF data file with IDL

The HDF data files can be read with IDL, for example with the routine `so2hdfread.pro`; this particular routine has been tested at IDL versions 6.0 and 6.3. Once the data has been read, it can be plotted (a simple example of that is provided), exported to other formats, etc.

==> [Return to HDF data format specification](#)

When running the example routine with the HDF file of the 3-day composite of 19-21 March 2007 [[HDF data file](#)] [[world plot of the SO2 slant column](#)], the output to the screen looks like this:

```
IDL> IDL> .run so2hdfread
IDL> so2hdfread

>>> Give the name of the HDF file to read
: data/so2cd2007031921.hdf

Product: SO2 column densities [DU] -- 3-day composite
No. of global attributes: 29
No. of datasets: 9

  id  Global Attribute (first six)
-----
  0  Product
  1  Data_version
  2  Creation_date
  3  Product_status
  4  SO2_field_date_1
  5  SO2_field_date_2

Details of the SO2_field_date_# attributes:

SO2_field_date_1 is of type LONG; no. of values:  3
SO2_field_date_2 is of type LONG; no. of values:  3

SO2_field_date_1 values stored : 2007    3    19
SO2_field_date_1 as a nice date: 19 March 2007

Number of longitudes, latitudes:    1440    720

Grid cell size (lon,lat):          0.250000    0.250000
First longitude value   :          -179.875
First latitude  value   :          -89.8750

Reading  Iscd_field data set ...
Skipping Iscd_error data set ...
Skipping Ivcd_field_1 data set ...
Skipping Ivcd_error_1 data set ...
Reading  Ivcd_field_2 data set ...
Skipping Ivcd_error_2 data set ...
Skipping Ivcd_field_3 data set ...
Skipping Ivcd_error_3 data set ...
Reading  Iccf_field data set ...

>>> Give a "return" to continue
:

Part of the data as example:
```

ilat	latitude	ilon	longitude	SCD [DU]	VCD [DU]	cloud frac.
500	35.125	1176	114.125	4.817	2.312	0.154
500	35.125	1177	114.375	4.761	2.316	0.139
500	35.125	1178	114.625	4.487	2.192	0.131

500	35.125	1179	114.875	3.551	1.771	0.104
501	35.375	1176	114.125	5.748	2.649	0.201
501	35.375	1177	114.375	6.321	2.843	0.220
501	35.375	1178	114.625	6.676	2.942	0.242
501	35.375	1179	114.875	4.835	2.284	0.151
502	35.625	1176	114.125	5.730	2.604	0.202
502	35.625	1177	114.375	8.064	3.359	0.330
502	35.625	1178	114.625	8.058	3.332	0.346
502	35.625	1179	114.875	6.255	2.781	0.227
503	35.875	1176	114.125	4.937	2.294	0.183
503	35.875	1177	114.375	7.240	2.968	0.365
503	35.875	1178	114.625	7.762	3.105	0.412
503	35.875	1179	114.875	7.013	2.940	0.322

```
>>> Extract the field value at a user-specified location
>>> Give the longitude, range: [-180:180] degrees;
    use 999 to end this extracting for values.
: -30
>>> Give the latitude, range: [-90:90] degrees
: 0
```

```
    Given coordinates fall in the grid cell with centre:
    longitude = -30.125
    latitude  = -0.125
    The SCD field value for this cell is: 0.455
```

```
>>> Extract the field value at a user-specified location
>>> Give the longitude, range: [-180:180] degrees;
    use 999 to end this extracting for values.
: 0
>>> Give the latitude, range: [-90:90] degrees
: 0
```

```
    Given coordinates fall in the grid cell with centre:
    longitude = -0.125
    latitude  = -0.125
    The SCD field value for this cell is -99, meaning that
    there is no data available for this grid cell
```

```
>>> Extract the field value at a user-specified location
>>> Give the longitude, range: [-180:180] degrees;
    use 999 to end this extracting for values.
: 0
>>> Give the latitude, range: [-90:90] degrees
: 30
```

```
    Given coordinates fall in the grid cell with centre:
    longitude = -0.125
    latitude  = 29.875
    The SCD field value for this cell is: 1.353
```

```
>>> Extract the field value at a user-specified location
>>> Give the longitude, range: [-180:180] degrees;
    use 999 to end this extracting for values.
: 999
```

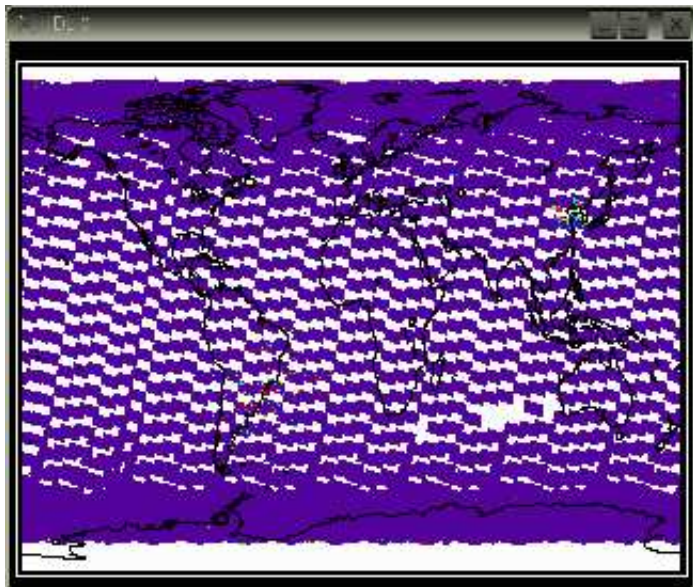
```
>>> Want to see a plot of the SO2 slant column field?
    Give "1" (one) for "yes" and something else for "no"
: 1
```

```
--- Plotting the SO2 slant column field, which takes a while ...
    The colour scale runs from 0.5 DU to 3 DU.
```

```
IDL>
```

The picture plotted by the routine is shown on the right. It uses a standard IDL colour table and is not ornamented with title, axis labels, etc.; it is merely meant as an example.

The part of the data set shown by the routine is right in the middle of a patch of large SO₂ values in the Air Quality SO₂ Service region "46. China"; see the [archive page](#) [at the website] for a close-up view.



Data and Services 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. Strictly speaking that number only applies to the data files based on SCIAMACHY measurements, not for OMI data as the production of OMI data is done by NASA/NOAA. This means that the addition of OMI data or changes therein does not change the version number. For that reason a separate 2-digit "service version number" S-## is used.

The version number of the processing looks like this: A.B.C

where A.B represents the version of the slant column retrieval and the notification system, and .C the version of the AMF-based vertical columns; if C is zero or absent, no vertical columns (VCDs) are available. See further down for a [list of VCD numbers](#).

The table below gives an overview of the version numbers and what was added/done for that version. Some additions to the website of the data record, which do not merit an increase of the version number, are added in the table for the benefit of the visitor who wants to track changes. Also additions of and changes to the OMI data are mentioned in the table.

version	date	history
1.0.3 S-07	January 2008	The colour scale of the SO ₂ vertical column plots in the archive has been adapted: it now ends at 2 DU (was 3), so that large SO ₂ values are better visible (the SO ₂ 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 S-06	November 2007	Near-real time images of OMI SO ₂ 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 S-05	August 2007	<p>Introduction of a new, improved background correction in the processing, in particular to try to get rid of most of the 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.</p> <p>A separate page gives a full overview of the new features of version 1.0.3.</p> <p>Initially, the archive covers the months January to June 2007; more data is added later.</p> <p>The near-real time processing and alert service were started on 16 August; the preceding days of that month were processed by hand as if in NRT.</p>
====> History of previous versions		

SCIAMACHY data version

The SCIAMACHY data, from which the SO₂ concentrations are derived, comes in different versions, depending on improvements in the official data processor and reprocessing of older data. The following table lists the software versions of the SCIAMACHY data used for the SO₂ retrieval available here. The cloud cover data used is FRESCO v5 and v5.1 (the latter starts in Dec. 2007).

<i>version</i>	<i>data period</i>
5.04	2004 : September -- December 2005 : January -- December 2006 : January -- 22 May
6.02	2006 : 22 May -- December 2007 : January -- 19 July
6.03	2007 : 19 July -- present

OMI data version

The OMI data, from which the SO₂ concentrations are derived by NASA/NOAA, comes in different versions, depending on improvements in the official data processor and reprocessing of older data. The following table lists the software versions of the OMI data used for the SO₂ retrieval available here; see [this page](http://disc.gsfc.nasa.gov/Aura/OMI/omso2.shtml) (<http://disc.gsfc.nasa.gov/Aura/OMI/omso2.shtml>) at the NASA website for details.

<i>version</i>	<i>data period</i>
002	17 August 2004 -- present

AMF & VCD data version

The last figure (C) of the data version number listed above refers to the version of the AMF-based vertical columns (VCDs) for the SCIAMACHY data; if C is absent it has value zero. The following table gives an overview of the versions.

C	date	info
0	--	No AMF and VCD are computed.
1	Nov. 2005 <i>was never implemented</i>	A preliminary version of AMF tables, using three different vertical SO2 profiles, based on yearly average SO2 data from anthropogenic activities ("air pollution profiles), for different SO2 concentration regimes. This was used for testing; results have not been made available.
2	May 2006 <i>was never implemented</i>	Similar to version '1', but with an extra vertical SO2 profile for very weak SO2 concentrations (the "no pollution case"), and one AMF table for each season. These tables have not been used.
3	March 2007 <i>implemented:</i> August 2007	AMF look-up tables with vertical profiles of an SO2 plume of 1 km thick at different altitudes for two types of SO2 concentrations: low (around 3 DU) and high (around 30 DU). For the processing three plume height are selected and used for computing the VCD, while one of these is used for the plots. <u>A separate page</u> provides more information.

Data and Services version history -- version 1.0.3

This page provides an overview of the new features of version 1.0.3 with respect to the previous version (0.9.0) in the processing and the data presentation on the web pages. The description is split into the following subsections:

- [General description](#)
- [SO₂ vertical column density](#)
- [Presentation on web pages](#)
- [Near-real time and Alert Service specific features](#)
- [Archive Service specific features](#)

For details on the different parts of the processing, consult the product information pages using the menu on the left.

General description

Due to the interference between the absorption signals of SO₂ and ozone, there were quite a lot of artifacts at high SZA, giving rise to "false alerts" in version 0.9.0. The background correction of version 0.9.0 (which was based on SO₂ as a function of SZA) was doing a reasonably good job for situations where the ozone distribution along a given longitude is more or less constant. In situations with large variations in the ozone concentrations, which in particular arise at high latitudes in Feb. - April at the Northern Hemisphere, the background correction was performing rather badly.

The new background correction is based on a relationship between the absorption signals of ozone and SO₂ and should therefore take into account automatically variations in the ozone concentration as function of longitude. This in itself already reduced the number of artifacts at high SZA considerably. A further improvement was found in some changes in the settings for the retrieval of the SO₂ slant column density.

The implementation of both the new retrieval settings and the new background correction implies that all data has to be reprocessed. This presented an ideal opportunity to implement some more improvements and additions to the service, such as the inclusion of SO₂ vertical column data and changes in the presentation of the data on the website.

The new background correction is doing a better job than the previous one, but there are -- and always will be -- artifacts at high SZA due to the interference in absorption signals. With the retrieval method currently in use (DOAS), it is probably not possible to make a more significant improvement to get rid of these artifacts and the corresponding "false alerts".

SO₂ vertical column density

Before only the SO₂ slant column density (SCD) was presented, but now also the SO₂ vertical column density (VCD) is given. The reason for adding the VCD is on the one hand that the VCD is a quantity that is more familiar to most people (it represents the total column density above the measurement point) and on the other hand to facilitate comparison with the results of other satellite-based measurements.

Please note that the values given for the SO₂ concentrations should not be taken as hard numbers. For the moment the SO₂ data -- in particular the VCD -- has not undergone a rigorous validation: only a qualitative and small-scale validation has been carried out so far.

In order to compute the VCD from the SCD, a so-called Air-Mass Factor (AMF) is used: $VCD = SCD / AMF$. And in order to determine AMF, information on the (effective) cloud cover fraction (CCF) is needed.

The AMF used here is based on pre-calculated look-up tables with a number of variables as entry points, such as viewing and zenith angles, as well as the height of the SO₂ plume. But the latter is not known from the retrieval in an automated processing, so an assumption must be made. It has been decided that the VCD is computed for three different assumed plume heights:

- 1 km above local ground level
- 6 km [or 1 km above local ground level, if that is higher]
- 14 km

The first one represents passive degassing of volcanoes and anthropogenic activities, the second one moderate volcanic eruptions and the third one explosive eruptions. These numbers agree more or less with the choice made by the OMI team for their SO₂ data retrieval and delivery.

All three VCDs based on these assumptions are available in the data files (which required a change in the data format of both the ASCII and the HDF data files), whereas the middle one is used for the plots presented on these web pages. The SCD is also plotted and can be accessed under "other plots".

The value of the AMF depends on the circumstances, but in most cases it will be larger than one, which means that the numerical value of the VCD will in most cases be lower than the numerical value of the SCD. At high SZA the AMF can be smaller than one, so that the VCD is larger than the SCD. The plots of both are made with the same colour bar, though. This means that a patch or large SO₂ that triggered an alert (which is based on the SCD) may not be so clearly visible in a VCD image.

Note that if no cloud cover information is available for a given ground pixel, the AMF and VCD of that ground pixel cannot be computed. In that case, the entries in the data files will get the "no data" value. Only the AMF for the clear-sky part will be given a value, as that can in principle be computed always.

Presentation on web pages

The pages presenting the data now show images of the SO₂ vertical column and the cloud cover fraction, and a plot of the region. A link is given to the plot of the SO₂ slant column and to the data file(s). To the left of the SCIAMACHY plot, the instrument name is mentioned: this is done because the intention is to add plots for the same regions using data from other satellite instruments.

The colour scale of the plots has been changed. The scale now starts at 0.5 DU, rather than zero, to reduce the low-level scatter of the background SO₂. The standard scale goes up to 3 DU, as before. But to easier identify really large SO₂ peak values, an additional colour has been added for values larger than 10 DU.

Apart from the plots for the set of geographic regions defined for the service, the previous version showed a plot for the whole world. As such a plot does not show the data near the poles very clearly, a "polar view" region has been added in the menu: it shows both poles in one plot, above (below) +30

(-30) degrees latitude.

Near-real time and Alert Service specific features

The dedicated web pages the alert notifications point to have been given a new layout. Previously such a page showed a plot of one or more geographic regions, depending on which regions crossed by the SCIAMACHY nadir state that issued the alert. This appeared to be rather confusing, especially because it was not always clear where the alerting nadir state lie. In the new version, a dedicated plot is made: a 30 by 30 degree region is drawn with the alerting nadir state right in the middle, and the plot shows only the data of the orbit that nadir state is part of. Below that a plot of the volcanoes (if there are any) in that dedicated region is shown.

If no cloud cover information is available, it is not possible to compute the AMF, and so the ground pixel in question would be marked as "no data". To have at least a rough idea of the VCD of that ground pixel, the NRT processing assumes that the ground pixel is cloud-free and uses the clear-sky AMF (which can be computed always) for the plots on the web page (not in the data file). Whether this happened can be seen from the absence of data in the plots of the cloud fraction.

Archive Service specific features

In the NRT service a VCD is shown assuming clear-sky conditions in case cloud cover data is missing (see above). This is not done for the archive service: if no cloud data is available, no AMF or VCD is available (the data files do contain - if possible - the value of the clear-sky AMF, but a "no data" value for the other parameters).

The archive service now also contains an overview of the alert cases of per month. This shows for which nadir states in the archive the criteria for "exceptional SO₂ concentrations" are met. The main table of the overview page is generated automatically, leaving room for remarks about the alert, e.g. about volcanic eruptions that may be related to the observed SO₂, based on external information. These remarks need to be added by hand, which takes time and so these pages are in a way always "under construction".

Data and Services version history -- pervious versions

Preceeding the version numbers listed at the main [Data and Services version history](#) page, the following versions have been available for SCIAMACHY data.

version	date	history
0.9.0 S-04	February 2007	<p><u>Automatic notification by e-mail</u> of "exceptional SO₂ concentrations" made public. The details of this service have not yet been incorporated in the on-line product information.</p> <p>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.</p>
	November 2006	<p>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.</p> <p>Update of the on-line product information, and offering the possibility to download that as one printable document; see the Documents section.</p>
	September 2006	<p>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.</p>
	June 2006	<p>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.</p> <p>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.</p> <p>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.</p> <p><i>Note that these improvements have changed the format of both the ASCII and the HDF data files.</i></p> <p>The documents that can be downloaded from the Downloadable documentation page are <i>not</i> yet updated to version 0.9.</p> <p><i>Later data additions for this version:</i></p> <ul style="list-style-type: none"> ● Slant column data and images for 2006: February, March, April ● Colour scale of cloud fraction plots improved.

0.8 S-03	November 2005	<p>Changes affecting only the ASCII data files of the SCD data at orbit coordinates:</p> <ul style="list-style-type: none"> ● Improved data file header (in preparation for addition of VCD data) ● Correction of the "relative azimuth angle" (error in previous version) <p>This does <i>not</i> affect the HDF data files or the images created before; they remain version 0.7.</p> <p>Other updates with this version:</p> <ul style="list-style-type: none"> ● Correction of the names of two regions that got mixed up ● Added slant column data and images for October 2005 <p><i>Later data additions for this version:</i></p> <ul style="list-style-type: none"> ● Slant column data and images for 2005: November and December; for 2006: January.
0.7 S-02	October 2005	<p>Full Volcanic & Air Quality SO₂ Archive Services set up, with:</p> <ul style="list-style-type: none"> ● Data files and images (daily, 3-day composites, monthly) of the SO₂ slant column for September 2004 to August 2005 ● 12 region defined for the Air Quality SO₂ Service ● Improved background correction ● Improved web access to the different archives ● More extensive product information ● Initial setup of criteria for the Notification Service of exceptional SO₂ emissions (not yet on the website) <p>Updates:</p> <ul style="list-style-type: none"> ● SO₂ slant column data and images of September 2005 added
0.6 S-01	December 2004 -- January 2005	<p>Prototype Volcanic SO₂ Archive Service set up, with:</p> <ul style="list-style-type: none"> ● Data of months September to November 2004 processed and plotted ● Special case page: Grímsvötn volcano eruption (1-2 Nov. 2004) presented ● Correction of background SO₂ levels applied to the DOAS retrieval of SO₂ slant columns ● Preliminary product information ● 41 regions, with lists and plots of volcano locations
-- S-00	mid 2004 and before	<p>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.</p>

Validation of the data products

Currently no real validation of SO₂ slant column or vertical column densities has been undertaken as yet. A problem is that there are few ground-based measurements of SO₂ that are appropriate for validation. It is planned to compare the results presented here with data from other satellite instruments. Furthermore, there is a close link with the [NOVAC project](#)[at the website], which intends to set up a network of ground-based stations for monitoring volcanic emissions of, among others, SO₂.

In setting up and fine-tuning the [SO₂ slant column \(SCD\) retrieval](#) with the DOAS method, the fitting results have been studied so as to optimise the settings for this retrieval. The slant columns have been compared to other results in an ad-hoc way for this, and in a few case studies. The SO₂ SCD values can thus be considered to be fairly accurate, but a more rigorous quantitative validation is necessary.

The SO₂ vertical column data (VCD) presented on the website are computed using an [air-mass factor using look-up tables](#) and an assumed height of the SO₂ plume. This approach provides only a rough estimate of the value of the VCD. Hence, the values given for the VCD should not be taken as hard numbers.

The [criteria for exceptional SO₂ concentrations](#) for the SO₂ data have been set up by examining the results of the retrieval and analysis processes. The results of alert events found by the processing are the source for the continuous (qualitative) validation of the alert service.

- In the near-real time service, the alert events are listed on dedicated web pages. At the bottom of these dedicated web pages there is room for adding notes and remarks, e.g. to link different alert to one and the same SO₂ event, to link to external information, etc. This has to be done by hand and is therefore done on an an-hoc basis.
- In the archive service, the processing provides an overview of alert cases for each month in the form of a table with some information on each SO₂ peak event found. Most of this table is generated automatically, but there is room to add remarks and other info by hand to each table.

[more to come]

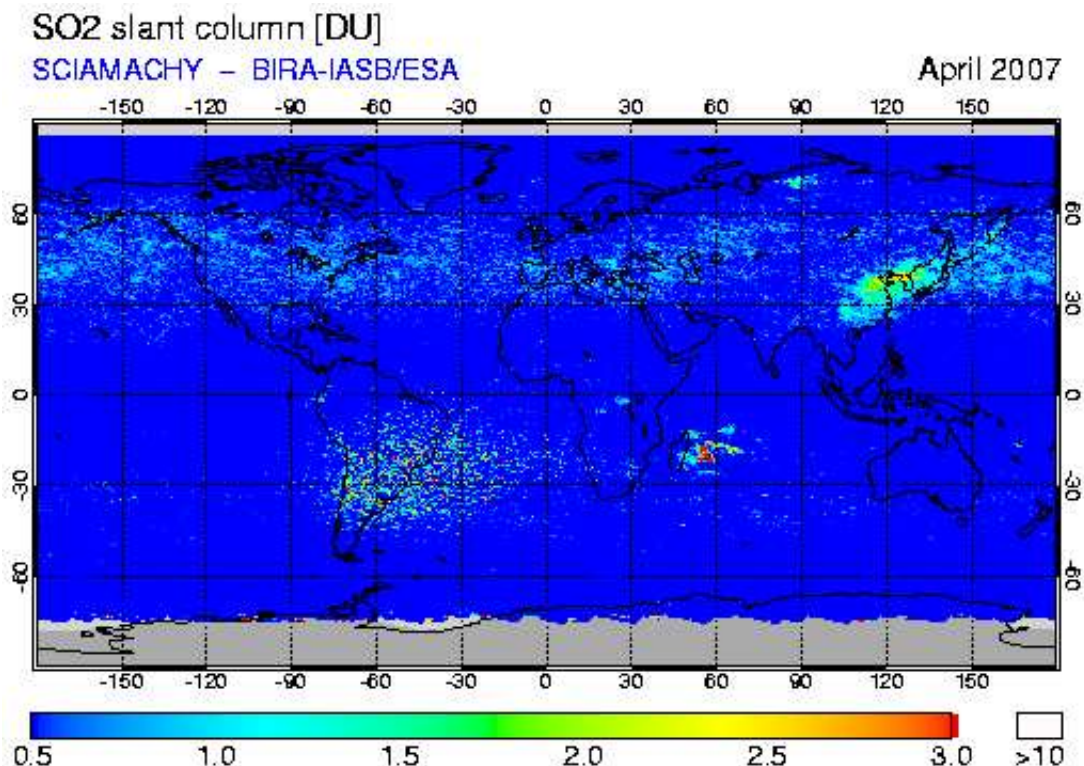
South Atlantic Anomaly

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 detector, causing higher-than-normal radiance values, which in turn decreases the quality of the measurements (*i.e.* the signal-to-noise ratio, of earthshine spectra), notably in the UV.

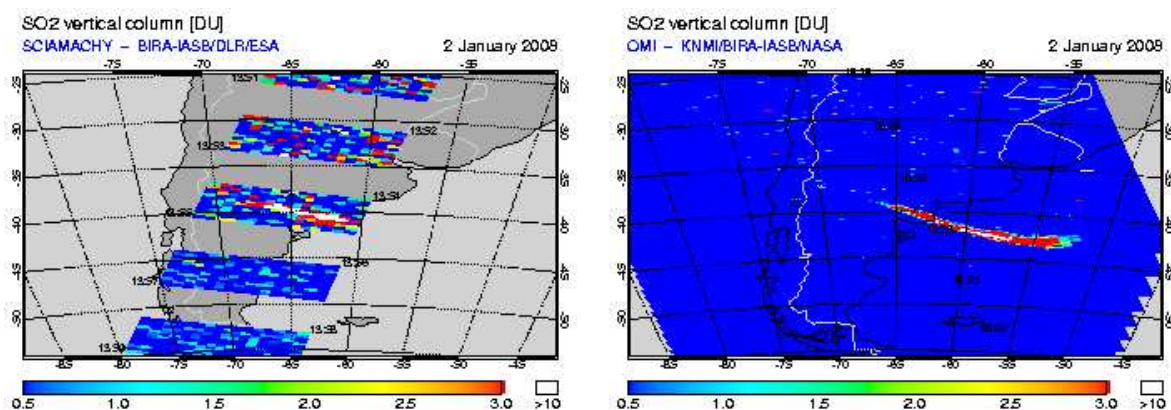
This reduction of the signal-to-noise also affects the retrieval of SO₂ slant columns: in the SAA region the variation in slant column values is much higher than elsewhere. This shows up clearly, for example, in the monthly average, as the image below illustrates. The decreased signal-to-noise may result in artifacts in the SO₂ slant columns.



The monthly average SO₂ slant column for April 2007. Note the increased noise in the SO₂ slant column over South America and a part of the Southern Atlantic Ocean, which can be attributed to the South Atlantic Anomaly.

SO₂ data derived from OMI measurement seem to be affected less by the SAA than GOME and SCIAMACHY. Probably this is because of the way the SO₂ is computed: as a kind of "by-product" of the ozone retrieval, and the ozone retrieval is less sensitive to the SAA due to the strong ozone absorption signals in the measurements.

Another difference is that SCIAMACHY and GOME are scanning instruments whereas OMI is an imaging instrument. A scanning instrument observes the individual ground pixels along an east-west swath one at a time and for each of these pixels charged particles will hit the detector in a different place and affect the measurements differently for each ground pixel. An imaging instrument sees an entire swath width in one go and there the detector is hit in several places by charged particles, affecting only a few ground pixels.



Example of SO₂ vertical column data based on SCIAMACHY (left) and OMI (right) data on 2 January 2008. The SO₂ plume is related to the eruption of the Llaima volcano (Chile), marked by a triangle in the OMI plot, on 1 January. The left plot shows a lot of noise in the SO₂ signal due to the interference caused by the SAA; the OMI data is clearly much less affected.

Because of these artifacts in the SO₂ data, neither the Volcanic SO₂ nor the Air Quality SO₂ Service has a geographic region defined in the area of the South Atlantic Anomaly for which plots are made and shown on the website. To benefit the analysis and to help avoid issuing false notifications of an exceptional SO₂ concentration due to the SAA, a "dummy region" of 40 by 40 degrees, centred around (-45.0,-25.0), is defined and monitored hidden from data users. This "SAA-region" overlaps with regions "Northern Chile" and "Central Chile" of the Volcanic SO₂ Service. As the following picture show, the "SAA-region" covers only the central part of the SAA, but for the moment this seems good enough.

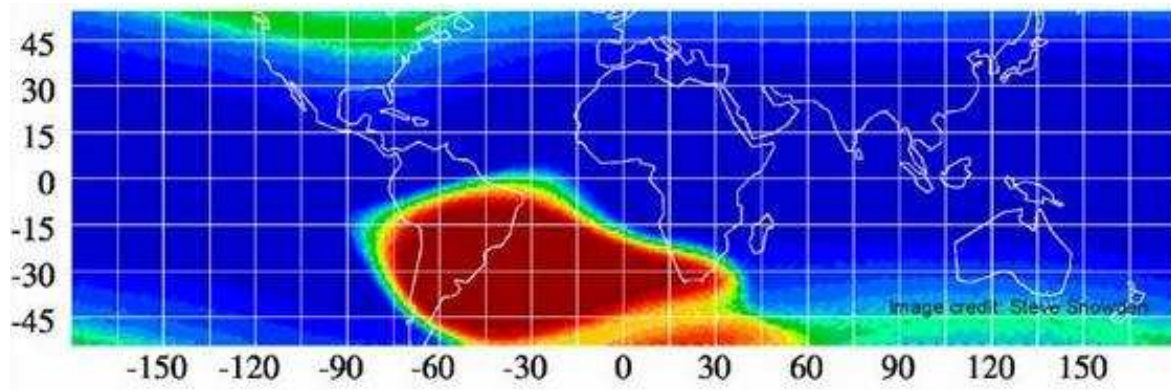


Image of the South Atlantic Anomaly from data collected by the X-ray detector of ROSAT. The image is taken from the [ROSAT page on the South Atlantic Anomaly](http://heasarc.gsfc.nasa.gov/docs/rosat/gallery/display/saa.html) (<http://heasarc.gsfc.nasa.gov/docs/rosat/gallery/display/saa.html>).

Downloading data & image files

This page gives some notes regarding:

- [Downloading data files](#)
- [Downloading image files](#)
- [High-resolution image files](#)

If you want to use data or images for a publication, in whatever form, please let us know!
We would like to keep a record of the usage of the data.

When using data or images, please mention by what instrument aboard which satellite the data was acquired, and that data and images can be found on the TEMIS website at <http://www.temis.nl/> (<http://www.temis.nl/>)

Downloading data files

The data files can all be downloaded by hand from the data archive access pages or from the data source given. This manual downloading is convenient for data from individual days or a few days.

For downloading many files you can send an email requesting the data and the files will be zip-ed together and made available for ftp-download.

Alternatively, use a script to call a program that can automatically download files from the web, such as "wget" (available [here](http://www.gnu.org/software/wget/wget.html) (<http://www.gnu.org/software/wget/wget.html>)):

```
wget [options] URL
```

or a text-based browser, such as "lynx" (available [here](http://lynx.browser.org/) (<http://lynx.browser.org/>)):

```
lynx -dump URL > output_file
```

Below follow some examples in the "wget" format, where

```
{DataPath}=http://www.oma.be/BIRA-IASB/Molecules/SO2archive/vs/
```

for short. For other sources of the data the URL is of course different; this one is valid for the SCIAMACHY data available via this website.

To download the HDF file with the daily gridded data for 17 June 2005:

```
wget {DataPath}/SciaDat/2005/06.hdf/17/so2cd20050617.hdf
```

To download the HDF file for the 3-day composite of 10-12 May 2005:

```
wget {DataPath}/SciaDat/2005/05.hdf/1012/so2cd2005051012.hdf
```

To download the HDF file for the monthly average of November 2004:

```
wget {DataPath}/SciaDat/2004/11.hdf/month/so2cd200411.hdf
```

To download the zip-ed ASCII data files for 26 September 2004:

```
wget {DataPath}/SciaDat/2004/09.dat/26/so2cd20040926.zip
```

To get access to a larger set of data files in one go, you can use the [data product contact](#) [at the website] to send in a request and the data files will be made available via anonymous ftp.

Downloading image files

The images (maps) presented on the website can be downloaded in a similar way as downloading the data files mentioned above.

Have a look at the images in the archive to see what the file names look like. Images of the slant column density start with `so2sc`, those of the vertical columns start with `so2vc`, and the cloud cover fraction images start with `ccf`. After that follows a string representing the date(s) and the region.

High-resolution image files

High-resolution images can be obtained from the [data product contact](#) [at the website] via email or anonymous ftp. When asking for high-resolution image, please specify:

- the format: PostScript, GIF, PNG, JPEG or TIFF
- if not PostScript, then *either* the size of the image in pixels, *or* the size of the image in cm or inch, as well as the resolution in dpi
- the date and region to plot
- the data type: daily data at orbit or grid coordinates, 3-day composite, monthly average
- whether you want the plot in colour (as on the web) or in a greyscale

Note that since these images have to be produced by hand, it is not possible to get a large number of images.

Downloadable documentation

Documentation on the Volcanic & Air Quality SO2 Services available for download:

- Printable version of the on-line product information, generated on 15 January 2008, which covers data product version 1.0.3 and service version S-07 (92 pages):
 - [zip-ed PS file \(1.7 MB; unzip-ed 34.7 MB\)](#)
 - [PDF file \(1.8 MB\)](#)

Note: when printing this document, the PS file gives slightly better images than the PDF file does, but in either case the images are not of high quality.

- Document [Sulphur dioxide monitoring within TEMIS](#), which covers data product version 0.9.0 [service version S-04], was delivered on 29 November 2006.

This document is primarily written to describe the SO2 data services within the themes "air pollution monitoring" and "support to aviation control" of the TEMIS project, but is intended to be more general and describe the SO2 data services as presented here for both the TEMIS and the PROMOTE project. The document is largely based on the on-line product information.

Presentations

- Poster "Monitoring of sulphur dioxide emissions from satellite as part of GSE PROMOTE" at the Atmospheric Science Conference, 8-12 May 2006, ESRIN, Frascati
 - [abstract submitted](#)
 - [poster as PDF file \(0.6MB\)](#)
 - [poster as GIF file](#)
- Oral presentation "Monitoring of volcanic activity from satellite as part of GSE PROMOTE" at the ESA ENVISAT symposium, 23-27 April 2007, Montreux
 - [PDF file of the proceedings paper \(6 pages; 365kB\)](#)

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List of acronyms

AMF	Air-mass factor
ASCII	American Standard Code for Information Interchange
BIRA-IASB	Belgian Institute for Space Aeronomy
BrO	Bromine monoxide
CGS	Carlo Gavazzi Space
DLR	German Aerospace Center
DOAS	Differential Optical Absorption Spectroscopy
DU	Dobson Unit
ECMWF	European Centre for Medium Range Weather Forecast
ENVISAT	Environmental Satellite
EOS-Aura	Earth Observing System - Chemistry & Climate Mission
ERS-2	European Remote Sensing satellite 2
ESA	European Space Agency
ESRIN	European Space Agency Research Institute
FRESCO	Fast Retrieval Scheme for Cloud Observables
GOME	Global Ozone Monitoring Experiment
GVP	Global Volcanism Program (at the Smithsonian Institute)
HCHO	Formaldehyde
HDF	Hierarchical Data Format
IDL	Interactive Data Language
KNMI	Royal Netherlands Meteorological Institute
MetOp	Meteorological Operational Satellite
MSG	Meteosat Second Generation
NASA	National Aeronautics and Space Administration
NO ₂	Nitrogen dioxide
NASA	National Oceanic and Atmospheric Administration
NOVAC	Network for Observation of Volcanic and Atmospheric Change
NRT	Near-real time
O ₃	Ozone
OMI	Ozone Monitoring Instrument
PROMOTE	Protocol Monitoring for the GMES Service Element: Atmosphere
SAA	South Atlantic Anomaly

SACS	Support to Aviation Control Service
SCD	Slant column density
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
SEVIRI	Spinning Enhanced Visible and Infrared Imager
SO ₂	Sulphur dioxide
TEMIS	Tropospheric Emission Monitoring Internet Service
TM	Chemistry Transport Model
TOMS	Total Ozone Mapping Spectrometer
VAI	Volcanic ash indicator
VCD	Vertical column density

Acknowledgments

The Volcanic & Air Quality SO₂ services are 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/>)

by the Belgian Institute for Space Aeronomy (<http://www.aeronomie.be/>) (BIRA-IASB, Brussels, Belgium) in collaboration with DLR (Oberpfaffenhofen, Germany) and KNMI (De Bilt, The Netherlands).

The TEMIS and PROMOTE projects are supported by the European Space Agency (<http://www.esrin.esa.it/>) (ESA).



The NRT Volcanic SO₂ Service is part of the Support to Aviation Control Service (SACS) (<http://sacs.aeronomie.be/>) of PROMOTE stage II.



Partners in SACS

BIRA-IASB Jos van Geffen, Michel Van Roozendael
Isabelle De Smedt, Caroline Fayt, Nicolas Theys

CGS Walter Di Nicolantonio, Lucia Tampellini
Giovanni Ballista, Alessandra Cacciari

DLR Pieter Valks, Thilo Erbertseder,
Klaus Wißkirchen

KNMI Ronald van der A

We would furthermore like to thank the following people for discussions, suggestions, information and other help:

<i>ESA-ESRIN</i>	Claus Zehner
<i>Météo France / Toulouse VAAC</i>	Philippe Husson, Patrick Josse
<i>RT Solutions, Inc.</i>	Rob Spurr
<i>UK Met. Office / London VAAC</i>	Claire Witham, Nigel Gait, Sarah Watkin
<i>University of Maryland / NASA</i>	Arlin Krueger, Simon Carn, Nick Krotkov
<i>US Geological Survey</i>	Marianne Guffanti

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