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Goddard Earth Science Data Information and
Services Center (GES DISC)

README Document for MSAQS02L4

A global catalogue of large SO₂ sources and
emissions Version 2

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1 Introduction

This document provides basic information about Version 2 of the global catalogue of emissions from large SO₂ point sources derived from the Ozone Monitoring Instrument (OMI) on NASA's EOS Aura spacecraft, the Ozone Mapping and Profiler Suite (OMPS) on the NASA–NOAA Suomi National Polar-orbiting Partnership (SNPP), and the TROPOspheric Monitoring Instrument (TROPOMI) on the ESA Copernicus Sentinel-5 Precursor (S-5P) spacecraft (Fioletov et al., 2022).

Sulfur dioxide (SO₂) slant column density (SCD) measurements from the three satellite instruments were used to detect large point emission sources or clusters of sources and estimate annual emissions from them. The sources were identified using different methods, including through OMI and TROPOMI SCD measurements utilized in the emission detection algorithm (Fioletov et al., 2016, McLinden et al., 2016; Theys et al., 2021), and their evolution was traced by estimating annual emissions from each source.

1.1 Dataset Description

The catalogue MSAQSO2L4 file contains the site coordinates, source type, country, source name, annual emissions, annual emission uncertainties, and the number of satellite pixels in the fitting area for three satellite instruments as well as for their weighted average.

1.2 Algorithm Background

The emission estimates are based on operational version 2 OMI and OMPS Principal Component Analysis (PCA) retrieval algorithm SO₂ SCD data (Li et al., 2020) as well as on new TROPOMI Covariance-Based Retrieval Algorithm (COBRA) SCD data (Theys et al., 2021). For this study, we have scaled constant SO₂ air mass factor (AMF) to a source-specific value based on such parameters as climatological surface reflectivity, surface pressure, average cloud fraction and pressure, and the SO₂ profile shape were also accounted for. As a result, a single time-independent site-specific AMF value for each site was calculated (McLinden et al., 2014) and applied consistently to each satellite SCD dataset to derive SO₂ vertical column densities (VCDs=SCDs/AMFs).

The emission estimate method for linking satellite-derived SO₂ VCDs to SO₂ emissions is based on a fit of satellite VCDs to an empirical plume model developed to describe the SO₂ spatial

distribution near emission point sources. The plume model assumes that the SO₂ concentrations emitted from a point source decline exponentially with distance and that they are affected by turbulent diffusion that can be described by a two-dimensional (2D) exponentially modified Gaussian function. The total SO₂ mass is derived from the fit and the emission rate is calculated as the ratio between the total mass and the prescribed SO₂ lifetime.

The algorithm for emission estimation is described by (Fioletov et al., 2015), the source detection algorithm is available from (McLinden et al., 2016). The original publication of the catalogue is (Fioletov et al., 2016). General information about SO₂ distribution and trends over different regions can be found in (Krotkov et al., 2016) and additional information about volcanic sources is available from (Carn et al., 2017).

Statistical uncertainties (one standard deviation, 1- σ) of the annual emission estimates are approximately 10 to 20 kt yr⁻¹ plus 5 % for 2005-2017, when the estimates were available from OMI and OMPS data only. These uncertainties are about 4-5 kt yr⁻¹ (1- σ) after 2018, when TROPOMI data are available. The uncertainties caused by the retrieval algorithms including AMF values are estimated at 50–60 %, but comparisons with reliable bottom-up inventories typically indicate agreement to better than 30% (based on the spread of the satellite estimated to reported emissions ratios).

1.3 Data Disclaimer

Data should be used with proper citation link:

Vitali Fioletov, Chris A. McLinden, Debora Griffin, Ihab Abboud, Nickolay Krotkov, Peter J. T. Leonard, Can Li, Joanna Joiner, Nicolas Theys, and Simon Carn (2022), Multi-Satellite Air Quality Sulfur Dioxide (SO₂) Sources and Emissions Database Long-Term L4 Global V2 , Greenbelt, MD, USA, Goddard Earth Science Data and Information Services Center (GES DISC), Accessed [**Data Access Date**]

<https://doi.org/10.5067/MEASURES/SO2/DATA406>

The attribution of the sources was done based on our best knowledge and may not always be correct. In some cases, there are several individual sources in close proximity, and it is difficult to estimate the contribution of each of them (Fioletov et al., 2017). For others, no definitive information was found on the source origin. Source identification from satellite data is particularly difficult in China, where point sources are numerous and are often located in clusters.

The emission estimation algorithm was developed for point sources. The fitting area size depends on the emission strength. For small sources, it is within a 90-km radius, so sources located 180 km

away do not affect emission estimates. The algorithm works reasonably well when there are two or even more sources in close proximity (20–30 km) but with no other sources nearby.

Information about such multiple sources can be found in the “Comment” column. We also added information on the distance to the nearest other source in the catalogue, so the users can do their own screening. In addition, to avoid “double counting” for regional emission estimates, some sources were not included in the catalogue if there is a source nearby that is already in the catalogue. This typically occurs in some regions of the US and China.

2 Data Organization

2.1 NetCDF-4 Product

The original Version 2 catalogue is contained in a Microsoft Excel file, but, within the framework of the MEaSUREs 2012 SO₂ project, these data have been converted into a netCDF-4 file. NetCDF-4 is a machine-independent, self-describing data format that is widely used for Earth Science datasets. The data hierarchy in a netCDF-4 file can be easily browsed with the HDFView tool (see “Tools for simple visualization” below). Conversion of the data to text format can be done using HDFView, or via other command-line utilities, such as h5dump or ncdump.

2.2 File Naming Convention

The file naming is fairly transparent:

```
MSAQSO2L4_2005-2021_v02-00.20221014.nc
```

This name states that the file is processing Level 4 (L4), the data range is “2005-2021”, the data/algorithm version is 2.00, and the file was produced on 2022-10-14.

As new data are added, the file is refreshed, and the file name, as well as the global attributes, are updated to reflect the new content.

2.3 File Format and Structure

The MSAQSO2L4 file is in netCDF-4, which is platform-independent. The structure can be visualized via the HDFView tool as global metadata and a hierarchy of data objects (see Figures 1 and 2). The key variables are described in Section 2.4 below.

The global attributes are attached to the MSAQSO2L4 netCDF-4 file at “root” level. They provide ample information regarding the Start/End time of the data inside the file, the version of the data, the Digital Object Identifier (DOI), etc. (see Figure 1).

General Attributes User Block		
Number of attributes = 41		
Name	Value	
AuthorAffiliation	ECCC, NASA/GSFC, BIRA-IASB, and MTU	
AuthorName	V.E. Fioletov, C.A. McLinden, D. Griffin, I. Abboud, N. Krotkov, P.J.T. Leonard, C. Li, J. Joiner, N. Theys, and S. Carn	
Conventions	CF-1.8	
DataSetQuality	The overall uncertainty is about 50%.	
DayNightFlag	Day	
EasternmostLongitude	180.0	
EndUTC	2021-12-31T23:59:59.999999Z	
Format	netCDF-4	
GranuleID	MSAQSO2L4_2005-2021_v02-00_20221014.nc	
IdentifierProductDOI	10.5067/MEASURES/SO2/DATA406	
IdentifierProductDOIAuthority	https://doi.org/	
InstrumentShortName	OMI, OMPS Nadir Mapper, TROPOMI	
LocalGranuleID	MSAQSO2L4_2005-2021_v02-00_20221014.nc	
LocalityValue	Global	
LongName	Multi-Satellite Air Quality Sulfur Dioxide (SO2) Database Long-Term L4 Global	
NorthernmostLatitude	90.0	
PGEName	MSAQSO2L4	
PGEVersion	2.0.0	
ParameterName	Estimated Annual Emissions Sulfur Dioxide	
PlatformShortName	Aura, Suomi-NPP, S5P	
ProcessingCenter	OMI TLCF	
ProcessingLevel	4	
ProductionDateTime	2022-10-14T02:00:00.000000Z	
RangeBeginningDate	2005-01-01	
RangeBeginningTime	00:00:00	
RangeEndingDate	2021-12-31	
RangeEndingTime	23:59:59	
SensorShortName	CCD Ultra Violet, Nadir Mapper, Imaging Spectrometer (Band 3)	
ShortName	MSAQSO2L4	
SouthernmostLatitude	-90.0	
StartUTC	2005-01-01T00:00:00.000000Z	
VersionID	2	
WesternmostLongitude	-180.0	
_NCProperties	version=2,netcdf=4.7.3,hdf5=1.8.19,	
comment	This release of the MSAQSO2L4 product is based on the Version 2 SO2 Emissions Catalogue by V. Fioletov, et al.	
featureType	timeSeries	
history	2022-10-14 02:00:00: original file produced in OMI TLCF	
institution	ECCC, NASA/GSFC, BIRA-IASB, and MTU	
references	https://doi.org/10.5067/MEASURES/SO2/DATA406	
source	OMI Aura, OMPS Nadir Mapper Suomi-NPP, TROPOMI S5P	
title	Multi-Satellite Air Quality Sulfur Dioxide (SO2) Database Long-Term L4 Global	

Figure 1. The global attributes in the MSAQSO2L4 netCDF-4 file, as represented by the HDFView tool (see “Tools for simple visualization” below).

The hierarchical structure of the MSAQSO2L4 netCDF-4 file is shown in Figure 2. The dimension variables are SourceIndex and Year. The groups are Catalogue, OMI_Aura, NPP_OMPS and S5P_TROPOMI. Each group contains four variables: Emissions, EmissionsSNR, EmissionsUnc and NumberOfPixels. The variables at “root” level are common to all groups: AMF, Elevation, Latitude, Longitude, NearestSourceDistance, NearestSourceIndex, NearestSourceName, OriginalSourceNumber, SourceComments, SourceCountry, SourceName, SourceType and Time.

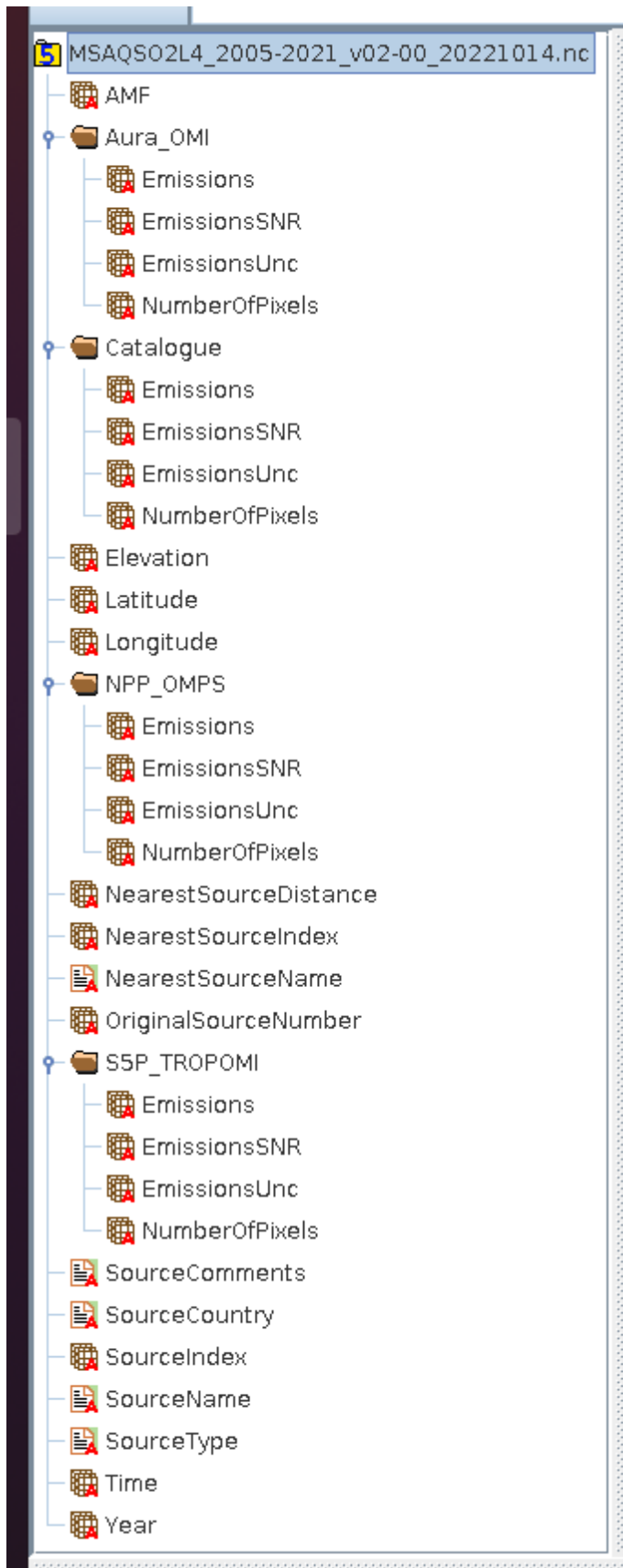


Figure 2. The dimensions, groups and variables in the MSAQSO2L4 netCDF-4 file as represented by the the HDFView tool (see “Tools for simple visualization” below).

2.4 Key Variables

<i>Variable</i>	<i>Content</i>
SourceIndex	The index for each source in the list of sources sorted by latitude (this variable is also a dimension).
Year	The (integer) year of the estimated emissions (this variable is also a dimension).
Latitude	The latitude of the source in degrees north (negative for the Southern Hemisphere).
Longitude	The longitude of the source in degrees east (negative for the Western Hemisphere).
Elevation	The source elevation above sea level in m.
Time	The (floating-point) mid-year time of the estimated emissions.
SourceType	The source type.
SourceName	The short name for the source identification.
SourceCountry	The country of the source location.
SourceComments	Additional information about the source. Note that the attribution of the sources was done based on our best knowledge and may not always be correct.
AMF	The Air Mass Factor (AMF) values used to adjust emissions based on the site elevation, albedo, etc. These post-processing AMFs can be different from the AMFs assumed in the Level 2 SO ₂ retrievals.
NearestSourceDistance	The distance to the nearest other source in the catalogue.
NearestSourceName	The name of the nearest source.
NearestSourceIndex	The index of the nearest source.
Emissions	The estimated emissions from the source in kt of SO ₂ per year.
EmissionsUnc	One standard deviation of the estimated emissions from the source in kt of SO ₂ per year.

EmissionsSNR	The ratio of estimated emission to the standard deviation of the estimate.
NumberOfPixels	The number of Level 2 pixels used for the fit for the smallest fitting area (30 km by 90 km). Note that larger fitting areas were used for large sources.
OriginalSourceNumber	The historical source number (for internal use).

2.5 Science Area

The catalogue presented herein can be used for verification of traditional (bottom-up) SO₂ emission inventories and identification of missing sources. It can be also used to fill gaps in available inventories, particularly if there are no other sources of information, e.g., for remote volcanoes. Conversely, those sites for which reliable SO₂ emission data are available can be used for OMI, OMPS, and TROPOMI SO₂ data product validation. The catalogue could also be used for cross-validation of different satellite data sources, similar to the comparison done for OMI, GOME-2, and SCIAMACHY (Fioletov et al., 2013). The catalogue could be particularly useful for the cross-validation of the new polar orbiting satellite instruments such as the European Commission Copernicus Programme Sentinel 5 (S5/TROPOMI), and the NASA-NOAA Joint Polar Satellite System (JPSS) OMPS nadir mappers. This could also be useful for the cross-validation of the next-generation geostationary satellites: GEMS (Geostationary Environment Monitoring Spectrometer) over Asia, TEMPO over North America in 2023, and Sentinel 4 over Europe in 2024.

3 Options for Reading the Data

3.1 Command Line Utilities

The HDF Group lists a number of HDF5 command line tools on their website:

http://www.hdfgroup.org/products/hdf5_tools/index.html#h5dist

Among them, the one that is the most useful for previewing HDF5 content is **h5dump**. The h5dump is the tool to use to have a very first look at any HDF5-formatted file, even if no documentation describing data is available. The tool by itself does not need extensive documentation, it is very straightforward to use and it's all options can be conveniently listed at the command line using the help option “-h”: h5dump -h

As of the current naming setup of the data fields, a simple list request “-n” will produce the following output, where full paths to groups and individual data fields (datasets) are obvious:

```
h5dump -n MSAQSO2L4_2005-2021_v02-00_20221014.nc
```

```
FILE_CONTENTS {
group   /
dataset /AMF
group   /Aura_OMI
dataset /Aura_OMI/Emissions
dataset /Aura_OMI/EmissionsSNR
dataset /Aura_OMI/EmissionsUnc
dataset /Aura_OMI/NumberOfPixels
group   /Catalogue
dataset /Catalogue/Emissions
dataset /Catalogue/EmissionsSNR
dataset /Catalogue/EmissionsUnc
dataset /Catalogue/NumberOfPixels
dataset /Elevation
dataset /Latitude
dataset /Longitude
group   /NPP_OMPS
dataset /NPP_OMPS/Emissions
dataset /NPP_OMPS/EmissionsSNR
dataset /NPP_OMPS/EmissionsUnc
dataset /NPP_OMPS/NumberOfPixels
dataset /NearestSourceDistance
dataset /NearestSourceIndex
dataset /NearestSourceName
dataset /OriginalSourceNumber
group   /S5P_TROPOMI
dataset /S5P_TROPOMI/Emissions
dataset /S5P_TROPOMI/EmissionsSNR
dataset /S5P_TROPOMI/EmissionsUnc
dataset /S5P_TROPOMI/NumberOfPixels
dataset /SourceComments
```

```
dataset /SourceCountry
dataset /SourceIndex
dataset /SourceName
dataset /SourceType
dataset /Time
dataset /Year
```

We can easily see which years and sources are included, in what order:

```
h5dump -d Year MSAQSO2L4_2005-2021_v02-00_20221014.nc
```

```
DATASET "Year" {
  DATATYPE H5T_STD_I32LE
  DATASPACE SIMPLE { ( 17 ) / ( 17 ) }
  DATA {
    (0): 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015,
    (11): 2016, 2017, 2018, 2019, 2020, 2021
  }
}
```

```
h5dump -d SourceName MSAQSO2L4_2005-2021_v02-00_20221014.nc
```

```
DATASPACE SIMPLE { ( 759 ) / ( 759 ) }
DATA {
  (0): "Nickel      ",
  (1): "Norilsk     ",
  (2): "Severonikel ",
  (3): "Severnyy, Vorkuta ",
  (4): "Usinsk-2    ",
  .
  .
  .
  (266): "Isdemir    ",
  (267): "Wuan        ",
  (268): "Xining      ",
  (269): "Baiyin      ",
  (270): "Matou      ",
  .
  .
  .
  (754): "Loy Yang    ",
  (755): "Villarrica  ",
```

```
(756): "Michael      ",  
(757): "Montagu     ",  
(758): "Erebus      "
```

In this example, there are 759 data sources, each source has a maximum of 17 year record.

Another very useful command line utility is **ncdump**. It is part of the netCDF distribution that needs to be compiled on the user's platform, but precompiled executables for Windows users do exist. The netCDF libraries are supported by the Unidata project at the University Corporation for Atmospheric Research (UCAR), and specifically the **ncdump** guide can be found at this location:

https://docs.unidata.ucar.edu/nug/current/netcdf_utilities_guide.html#ncdump_guide

The options that most likely would be used are “-h” for global view of netCDF files data fields and their attributes, dimensions, and file global attributes.

Another frequently used option is “-v” for previewing of science values in the data fields.

3.2 Tools for simple visualization and file content view

3.2.1 HDFView

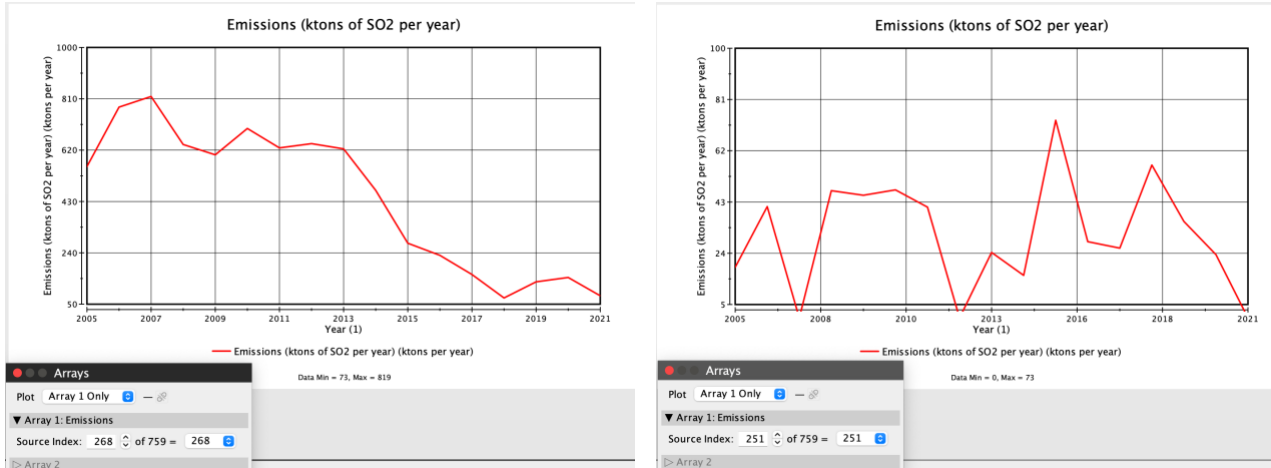
Among the interactive (with user interface) HDF tools, **HDFView** is one of the simplest to use and install on your local desktop. Strength of HDFView is that it is good for all HDF and netCDF formats. Another strength is that file content is presented graphically in a very friendly fashion – all data groups are presented as folders, where user can easily drill down the file hierarchy, which is especially useful for HDF5. Numerical data sets can be viewed as spreadsheets, and as images (multidimensional datasets). Simple data manipulations are possible. For download and more information, follow this link:

<http://www.hdfgroup.org/hdf-java-html/hdfview/index.html>

3.2.2 Panoply

The Panoply tool, developed at the Goddard Institute for Space Studies (GISS), is a simple tool with intuitive interface to scout data content and make simple plots. Since MSAQSO2L4 represent

point sources, and data are not organized primarily by longitude and latitude, maps cannot be produced. Still, it is very easy to check sources names (locations) and their indices, and make time plots at a given location as shown below. Selected is Emissions data from the Aura_OMI folder, and the source index in Panoply is 1-based. The scale for South Korea is manually set to be 10 times smaller than the Wuan plot.



Wuan, China

Yeongheung, South Korea

3.2.3 Commercial

IDL and MatLAB, are two major commercial data languages, coming with their libraries that fully support all HDF formats. The HDFEOS group has added simple IDL and MatLAB recipes on their web site in particular for GSSTF data in the HDF-EOS5:

http://hdfeos.org/zoo/index_openGESDISC_Examples.php

4 Data Services

4.1 GES DISC User Interface

GES DISC provides new advanced keyword, spatial, and temporal searches, as well as advanced web services (like OPeNDAP), through its interface. To directly find this particular dataset:

<https://disc.gsfc.nasa.gov/datasets?keywords=MSAQSO2L4>

Users don't have to memorize exact dataset names. It would suffice to enter some relevant keywords, like "SO2 meas" to find this and other SO₂ datasets, mostly relevant to the MEaSURES project:

<https://disc.gsfc.nasa.gov/datasets?keywords=so2%20meas>

Also possible:

<https://disc.gsfc.nasa.gov/datasets?keywords=so2%20volcano>

4.2 Earthdata Search

Use Earthdata Search Client (EDSC) to find and retrieve data sets across multiple data centers. A shortcut to search for MSAQSO2L4 would be:

<https://search.earthdata.nasa.gov/search?q=MSAQSO2L4>

4.3 OPeNDAP

OPeNDAP stands for "Open-source Project for a Network Data Access Protocol". OPeNDAP is a framework that simplifies all aspects of scientific data networking. It provides simple means for parameter and spatial subsetting. The spatial subset is actually a subset by array index - array being the grid data. In the most simplistic case, OPeNDAP can be used to convert data from HDF-EOS5 to ASCII. The data directory hierarchy, of all MEaSURES-related SO₂ data sets, as served by OPeNDAP, can be viewed in any browser:

<http://measures.gsfc.nasa.gov/opendap/SO2/contents.html>

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