P1.8 ATMOSPHERIC COMPOSITION DATA PRODUCTS FROM THE EOS AURA MLS

Suraiya P. Ahmad *[1], Joe Waters[2], James Johnson[1], Irina Gerasimov[1], Gregory Leptoukh[1], Steve Kempler[1]

[1]Goddard Earth Sciences Data and Information Services Center (GES DSIC)
NASA Goddard Space Flight Center, Greenbelt, MD

[2]NASA Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA

1. INTRODUCTION

To improve the understanding of atmospheric chemical and dynamic processes, sources and sinks of tropospheric pollutants, coupling of upper troposphere and lower stratosphere and how changes in atmospheric constituents affect air quality and climate, the Microwave Limb Sounder (MLS) was launched on the Earth Observing System (EOS) Aura Satellite on 15 July 2004. MLS provides day and night global measurement of vertical profiles of several atmospheric chemical constituents (O_3, HCl, ClO, HOCl, BrO, OH, H_2O, HO_2, HNO_3, N_2O, CO, HCN, CH_3CN, volcanic SO_2), cloud ice, geopotential height, and temperature of the atmosphere. The EOS-Aura MLS is an improved version of the successful UARS MLS experiment with better spatial resolution and coverage, extended vertical range, and capability of measuring some new chemical constituents (OH, HO_2, and BrO) never measured before globally from space. Ozone (a tropospheric pollutant), carbon monoxide (a good tracer of anthropogenic pollution) and HCN & CH_3CN (biomass burning tracers) will help in quantifying aspects of pollution in the upper troposphere (Waters et al., 2006).

EOS Aura carries three other instruments Ozone Monitoring Instrument (OMI), High Resolution Dynamics Limb Sounder (HIRDLS) and Tropospheric Emission Spectrometer (TES). These four instruments provide simultaneous observations of the same atmosphere but in different spectral regions and at different vertical resolutions. Aura MLS measurements, in conjunction with the measurements from the other Aura instruments, will help in improving the understanding of stratospheric and tropospheric chemistry. EOS MLS began its full atmospheric science observations on 13 August 2004, with excellent performance to date in all portions of the instrument. After preliminary validation (Froidevaux et al., 2006), the MLS Version 1.51 data are now publicly available. The Aura MLS and OMI derived geophysical atmospheric composition data products are archived at NASA Goddard Earth Sciences Data and Information Services Center (GES DISC) and are available free (http://acdisc.gsfc.nasa.gov) to the public. In the near future HIRDLS data will be also made available from the GES DISC.

For the atmospheric chemistry data archived, GES DAAC provides customized data search mechanism; subsetting capabilities (with selection criteria of bands, parameters, and geographical region); and visualization capabilities through Giovanni, a web-based on-line data visualization tool with an option of image display or ASCII output (http://acidsc.gsfc.nasa.gov/tool.shtml).

This presentation provides an overview of the MLS standard and diagnostic data products. Brief details of the MLS data support activities are also presented. MLS related publications are available from the MLS project web site http://mls.jpl.nasa.gov.

2. MLS INSTRUMENT

The MLS instrument flown on Aura spacecraft orbits in a 705 km, 98.2-degree inclination and sun-synchronous polar orbit (98.8 minute period), with an equatorial crossing time (ascending node) of 1:45 pm. The MLS field-of-view looks in the forward direction (direction of orbital motion) and vertically scans the Earth's limb (in the orbital plane) from the stratosphere into the upper troposphere, in 20 seconds, in five spectral regions centered at 118, 190, 240, 640 GHz and 2.5 THz. This is followed by about 5 s of antenna retrace

* *Corresponding author address:*
Suraiya P. Ahmad, NASA GSFC, Code 610.2,
Greenbelt, MD 20771;
e-mail: ahmad@acdisc.gsfc.nasa.gov

and calibration activity. The vertical scans at every 25 seconds are spaced 1.5° (about 165 km) along the orbit track. This gives 82 deg south to 82 deg north latitude coverage on each obit (240 scans per orbit). MLS obtains vertical scans at 3500 locations over the globe every 24 hours (Waters et al., 2006).

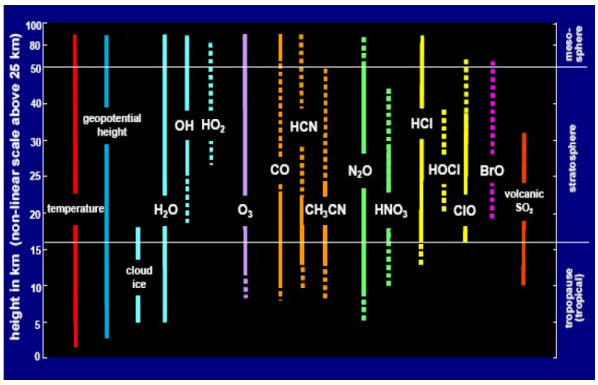


Fig.1. EOS MLS Atmospheric Measurements. Solid lines indicate generally useful precision for individual profiles. Dotted lines indicate that zonal (or other) averages are generally needed to obtain useful precision. Solid lines for lower stratospheric and upper tropospheric HCN and CH3CN apply to enhanced abundances expected from biomass burning injections. The height ranges shown here indicate what is ultimately expected to be achieved, and not necessarily achieved with the current version of data processing. Different colors indicate different chemical families. (Courtesy of J. Waters, MLS Principal Investigator).

3. MLS DATA PRODUCTS

MLS provides day and night global measurement of vertical profiles of several atmospheric chemical constituents (O_3, HCl, ClO, HOCl, BrO, OH, H_2O, HO_2, HNO_3, N_2O, CO, HCN, CH_3CN, and volcanic SO_2), cloud ice, geopotential height, and temperature of the atmosphere (Fig. 1). MLS data products are available at four processing levels Level 0, Level-1B, Level-2, and Level-3. Level-0 products consist of raw instrument data at original resolution, time ordered, and duplicate packets removed. Level-0 data are further processed to convert counts to radiometric calibrated radiances and produce Level-1B products. The Level-1B calibrated radiances are then used to produce geophysical data products (Levels-2 & 3). MLS Level 0, Level-1B & and Level-2 products contain data from 15 orbits (data points spaced 1.5 degree, about 165km, along the orbital track), whereas Level-3 products contain data that are averaged over time (daily or monthly) for small equal angle (latitude x longitude) grids covering the whole globe (Cuddy et al., 2006). MLS Level-1B and Level-2 data files also contain temporal, spatial, and viewing geometry parameters, and several quality flags, in addition to the standard retrieved geophysical parameters.

Though detailed validation of the MLS products is still underway, the version 1.51 Level-2 data products are considered suitable for general scientific use and are released to the scientific community. These data are archived at the GES DISC and available free to the public (http://acdisc.gsfc.nasa.gov/Aura/MLS/data_products.shtml). The Level-3 products will be available in the near future.

The Level-1B files are in HDF5 Swath format, Level-2 files are in HDF-EOS5 swath format, and Level-3 files are in HDF-EOS5 Grid or Zonal Mean format. Data read software and tools, with the option of browsing capability and ASCII output, are also made available from the GES DISC DAAC (http://acdisc.gsf.nasa.gov/tools.shtml).

Brief details of the MLS products are given below.

3.1 MLS Radiometrically Calibrated Radiance Products (Level-1B)

The radiometric calibration measurements (MLS views of on-board blackbody calibration targets and/or cold space) are acquired between each limb scan (every 25 seconds). The “Level - 1B Algorithm” is used at to produce Level-1B MLS products. It takes the raw sensor measurements (Level-0 data), calibration and spacecraft ephemeris information and produces accurate radiometrically calibrated radiances (Jarnot et al., & Pickett et al., 2006). Four types of Level-1B standard products (see Table 1) are produced.

Table 1 - Level 1B Radiance Products

(File Format HDF5)

Short Name	Description	MLS Contact
ML1OA	Orbit/Attitude and Tangent Point Geolocation Data	Robert Jarnot jarnot@jol.nasa.gov
ML1RADD	Radiances from Digital Autocorrelators	
ML1RADG	Radiances from Filter Banks for GHz	
ML1RADT	Radiances from Filter Banks for THz	

3.2 MLS Level-2 Geophysical Products (L2GP)

The calibrated radiances (Level-1B data) and ancillary information, operational meteorological data from GMAO (NASA’s Global Modelling and Assimilation Office) or NCEP (National Centers for

Environmental Prediction) are used in the 'Level-2 Algorithm' to retrieve vertical profiles of atmospheric constituents (O_3, HCl, ClO, HOCl, BrO, OH, H_2O, HO_2, HNO_3, N_2O, CO, HCN, CH_3CN, and volcanic SO_2), cloud ice, geopotential height, and temperature of the atmosphere (Fig. 1) for each data point, spaced 1.5° (about 165 km) along the orbit track (3500 profiles per day). The 'Level 2' retrieval algorithm (Livesey et al., 2006) is based on a standard 'Optimal Estimation' retrieval approach (Rodgers, 1976) that seeks the "best" value for the state vector (the profiles of temperature and species) based on an optimal combination of the fit to, the MLS radiance observations, *a priori* estimates of the state vector (from climatological fields), and constraints on the smoothness of the result.

Standard and Diagnostic Products – MLS Level-2 retrieval algorithm produces two types of products, the standard and diagnostic products (see Tables 2a & 2b). The contents in these files are similar. However, the retrievals for the diagnostic products has typically been obtained using radiances from a different spectral region (i.e different radiometer) than that used for the standard products.

Each Level-2 product file contains two main retrieved geophysical parameters ('L2gpValue' and 'L2gpPrecision' data field) for the vertical scans made in 24 hours. In addition to the mixing ratio of the atmospheric constituents or temperature profiles, these files also contain geolocation information (latitude, longitude, tanget height), time and quality flags.

The quality of each retrieval is indicated by three data fields 'L2gpPrecision' (Estimated Precision), 'Quality ', and 'Status'. For the detailed information about the quality of measurements of each species, including recommended pressure ranges, and quality thresholds, please refer to the detailed 'Version 1.5 Level 2 data quality and description document' and the 'supplement document' produced by the MLS instrument team and available from MLS and GES DISC sites

http://mls.jpl.nasa.gov/ & http://acdisc.gsfc.nasa.gov/Aura/documentation/ .

Column abundance - The standard product data files for the atmospheric constituents include an additional 'HDF-EOS5' swath containing an integrated column abundance of the product above the tropopause. These are named such as 'column O3' or 'column BrO'.

Table 2a- MLS Level-2 Standard Data Products

(File Format HDF-EOS5 Swath)

Product	Short Name	Useful vertical range hPa	MLS contact
*BrO	ML2BrO	10 - 2.2	Nathaniel Livesey livesey@mls.jpl.nasa.gov
ClO	ML2CLO	100 – 1.0	Michelle Santee mls@mls.jpl.nasa.gov
CO	ML2CO	215 - 0.0046	Mark Filipiak M.J.Filipiak@ed.ac.uk
Geopotential Height	ML2GPH	316 - 0.001	Michael Schwartz michael@mls.jpl.nasa.gov
H_2O	ML2H2O	316 - 0.1	**troposphere:** Bill Read bill@mls.jpl.nasa.gov **stratosphere:**Hugh Pumphrey H.C.Pumphrey@ed.ac.uk
HCl	ML2HCL	100 - 0.22	Lucien Froidevaux lucien@mls.jpl.nasa.gov
HCN	ML2HCN	10 - 1.4	Hugh Pumphrey H.C.Pumphrey@ed.ac.uk
HNO_3	ML2HNO3	147 - 3.2	Michelle Santee mls@mls.jpl.nasa.gov
*HO_2	ML2HO2	22 - 0.22	Herb Pickett hmp@jpl.nasa.gov
*HOCl	ML2HOCL	22 - 2.2	Lucien Froidevaux lucien@mls.jpl.nasa.gov
Ice Water Content	ML2IWC	215 - 68	Dong Wu dwu@mls.jpl.nasa.gov
N_2O	ML2N2O	100 - 0.1	Nathaniel Livesey livesey@mls.jpl.nasa.gov
O_3	ML2O3	215 - 0.46	**troposphere**: Mark Filipiak M.J.Filipiak@ed.ac.uk **stratosphere**: Lucien Froidevaux lucien@mls.jpl.nasa.gov
OH	ML2OH	46 - 0.22	Herb Pickett hmp@jpl.nasa.gov
Relative Humidity	ML2RHI	316 - 0.1	Bill Read bill@mls.jpl.nasa.gov
Temperature	ML2T	316-0.001	Michael Schwartz michael@mls.jpl.nasa.gov
Volcanic SO2	ML2SO2	316-0.001	Bill Read bill@mls.jpl.nasa.gov

Products with a * require significant averaging over most or all of their vertical range in order to obtain a useful signal-to-noise ratio (Source: J. Waters, 2006)

Table 2b - Level 2 Diagnostics Products

Short Name	Description
ML2GP-DGG	Level-2 Diagnostics, Geophysical Parameter Grid (in HDF-OES5)
ML2AUX-DGM	Level-2 Diagnostics, Miscellaneous Grid (in HDF5)

3.3 MLS Global Gridded Products (Level -3)

The standard Level-3 products are Daily Gridded Maps (separate file corresponding to each Level-2 product), Monthly Gridded Maps, Daily Zonal Means and Monthly Zonal Means (see Table 3a and 3b). The Level-3 products will be available in near future.

Table 3a - Level 3 Gridded Products

(File Format HDF-EOS5: Grid Format)

Short Name	Description
ML3D<XX>	Level-3 Gridded Daily Maps; separate file for each Level-2 <XX> product for which Level-3 map is produced
ML3DSPC	Level-3 wave spectra for each map: Fourier components fitted to the Level-2 data (amplitude and phase for each latitude and pressure level ; 10 days entered on ~30days of Level-2 data)
ML3MMAPS	Level-3 Monthly Maps, Standard Products
ML3MMAPD	Level-3 Monthly Maps, Diagnostic Products

Table 3b- Level 3 Zonal Mean Products

(File Format HDF-EOS5: Zonal Mean Format)

Short Name	Description
ML3DZMS	L3 Daily Zonal Means, Standard Products
ML3DZMD	L3 Daily Zonal Means, Diagnostic Products
ML3MZMS	L3 Monthly Maps, Standard Products
ML3MZMD	L3 Monthly Maps, Diagnostic Products
ML3MMAPS	L3 Monthly Maps, Standard Products
ML3MZMD	L3 Monthly Maps, Diagnostic Products

3.4 File Naming Convention

For Level-2 products, the standard product files are named according to the convention:

MLS-Aura_L2GP-<product>_v01-51-cxx_<yyyy>d<ddd>.he5

Where <product> is the parameter (e.g. BrO, O3, Temperature, etc); <yyyy> is four digit calendar year, <ddd> is Julian day in that year. The file contains an HDF-EOS swath given the same name as the product.

The Level-2 Diagnostic files are named as:

MLS-Aura_L2GP-DGG_v01-51-cxx_<yyyy>d<ddd>.he5

MLS-Aura_L2AUX-DGM_v01-51-cxx_<yyyy>d<ddd>.h5

'cxx' is cycle number 'xx' (it indicates that the file is generated at times other than the usual expected time because of some system problem or delay in ancillary files)

The Level-3 files are named as:

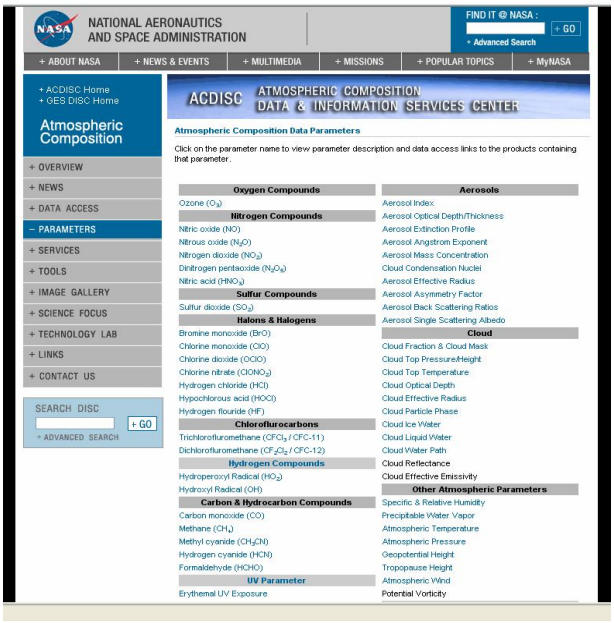
MLS-Aura_ ML3D<xx>,

Where xx is Level-2 product which is used in producing Level-3 maps.

4. MLS DATA PRODUCT SUPPORT FROM THE NASA GES DISC DAAC

The Atmospheric Composition Data Support Team at the GES DISC provides assistance to the user in the areas of accessing data products, documentation, browse, and data analysis software. Brief details of the data support activities are provided below.

4.1 Atmospheric Composition Data and Information Services Center (ACDISC) – ACDISC is a virtual data center which is established at GES DISC (Leptoukh et al, 2005) . It provides a comprehensive atmospheric composition database, which consists of data from several solar occultation, limb, and nadir imaging satellite based sensors that are archived at the GES DISC and data residing at other remote data centers. It also provides web-based data subsetting and data visualization capabilities for the atmospheric composition data available from ACDISC. Some key atmospheric composition datasets residing at the GES DISC available through ACDISC (http://acdisc.gsfc.nasa.gov/) are from Aura MLS, OMI, HIRDLS; UARS HALOE, MLS, CLAES, ISAMS, MODIS & AIRS; LIMS, TOMS, SBUV & BUV; SSBUV & ATMOS; and GOME (mirror site) sensors.



4.2 A-Train Data Depot (ATDD) - ATDD is another virtual data portal/center which is established at the GES DISC to process, archive, provide access, visualize, analyze and correlate distributed atmosphere measurements from various A-Train instruments along A-Train tracks. The succession of US and international satellites that follow each other, seconds to minutes apart, across the local afternoon equator crossing is called the A-Train. The A-Train consists of the following satellites, in order of equator crossing: OCO (to be launched in 2008), Aqua, CloudSat and CALIPSO (to be launched in near future), PARASOL, and Aura Data from A-Train are combined to create a consolidated, synoptic, vertical view of the Earth's Atmosphere (http://disc.gsfc.nasa.gov/atdd/). Aura MLS and Aqua AIRS Temperature Profile along the CloudSat track for 06/21/05, 12:00 to 12:50 GMT are shown in Fig.2. The collocated curtain plots can be useful in the data validation activities.

4.3 MLS Giovanni for the ACDISC & ATDD

The Giovanni (GES-DISC Interactive On-line Visualization & Analysis Infrastructure) is a Web based interface for data exploration, visualization and analysis. It has been developed to provide an easy access to the long-term atmospheric composition datasets residing at the GES DISC virtual Atmospheric Composition Data and Information Services Center (ACDISC) and A-Train Data Depot(ATDD).

Giovanni facilitates science data usage by providing data exploration capabilities based on user requested criteria. There is no need to learn data formats, everything is done via a web browser. User can save the images generated during the data exploration session and download the subsetted data in ASCII (option of download of data in original format is also available).

Several plot type options are available depending on the mission and the parameters selected.

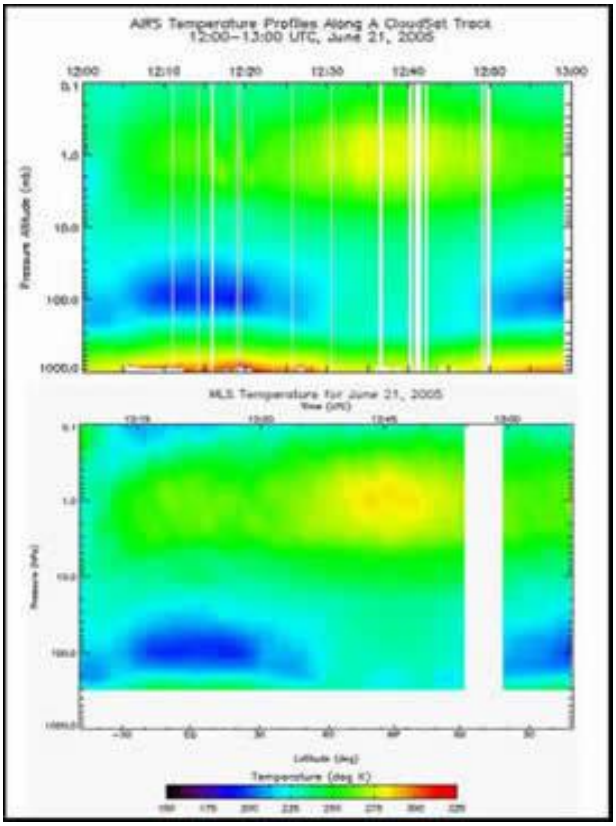


Fig. 2 Aqua AIRS (top) and Aura MLS (bottom) Temperature profiles along a CloudSat track for June 21, 2005, 12:00 to 12:50 GMT.

For example for almost all gridded products (Level-3 data) the available plot types are: 2D maps for spatial distribution, maps of latitudinal or longitudinal distribution as a function of time also referred as Hovmoller plots, time-series along with simple statistics, animations, meridional and zonal averages, multi parameter comparisons, scatter plots, correlation maps, maps of differences for the parameters from two different sources.

For Aqua AIRS, Aura MLS and UARS HALOE data, the Giovanni provides browsing capabilities of vertical profiles of trace gases, temperature and geopotential height.

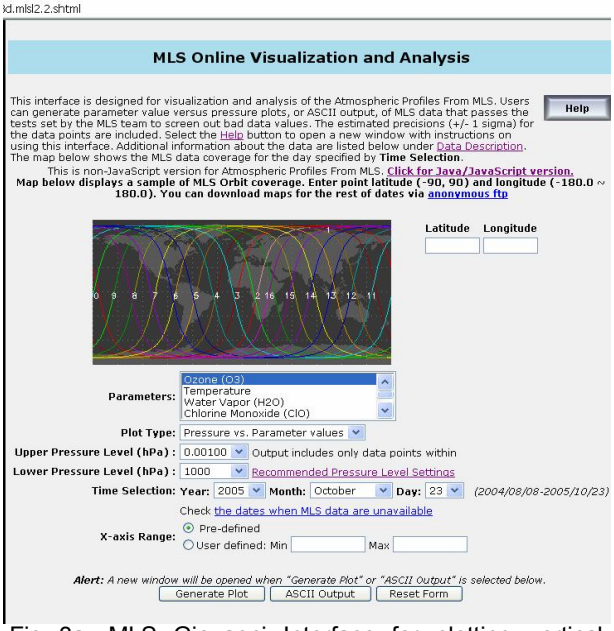


Fig 3a. MLS Giovanni Interface for plotting vertical profiles and precision estimates.

Based on the user selected latitude and longitude values, MLS Giovanni generates parameter values vs. pressure plots for the data within 500, or 1000 km of selected site. Only those data are shown that pass the quality criteria set by the MLS science team to screen out bad values. For example, data with positive estimated precision, 'status' equal to zero and 'quality' equal to or higher than the thresholds are only displayed). The estimated precisions (+/- 1 sigma) of the data points are also plotted. The option of ASCII output is available. Figure 3a (above) shows MLS Giovanni user interface and Fig 3b (bottom) shows plots of three nearest profiles.

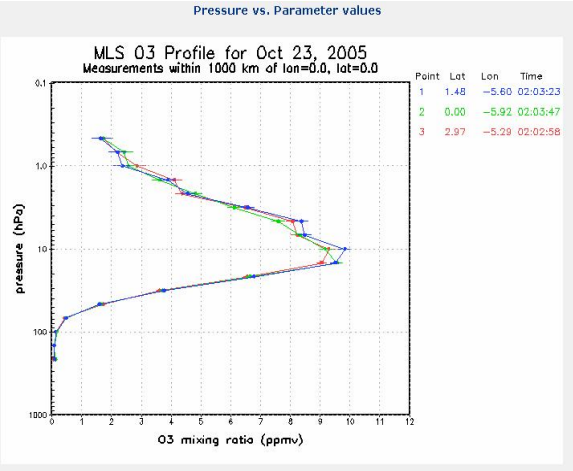


Fig 3b. Plots of MLS ozone profiles with+/- one sigma bars. Three profiles are shown that are closest to the selected site on the map.

4.4 Data Read Software for MLS Products

MLS data sets archived at NASAGES DAAC are in the HDF-EOS5 (Hierarchical Data Format-Earth Observing System) based on HDF5 format. This format has been adopted by NASA for standard data product distribution since it is able to handle multiple types of data objects and at the same time is independent of the platform or operating system the file is created on. MLS Level 1B data files (radiances and calibration files) are written in HDF5 format and MLS Level-2 products (derived geophysical parameters) are written in HD-EOS5 format and the file names have extension '.h5 ' and '.he5,' respectively

For convenience, 'Read Software' and data analysis tools have been developed by the GES DSIC Data Support Team in C, Fortran, and IDL languages (http://acdisc.gsfc.nasa.gov/tools.shtml) These software are capable of data extraction, subsetting, analysis, reprojection, and format conversion (binary or ASCII file). Some software are command line programs consist of only few lines and users can easily insert in their data analysis code.

ACDISC provides two data read software (interactive command-line programs) '**read_h5**' and '**atmos_h5**', for the MLS and other Aura data files.

read_h5: It is written in the C language. The program displays tree structure of the data objects and allows users to select a parameter, latitude range, and dump the data in ASCII.

atmos_h5: It is an IDL based code (works with IDL version 6.1 or higher). This program not only provides the parameter subsets and options of ASCII or binary output, it also displays quick look image and creates jpeg file.

4.5 GES DISC HDF-EOS5 Subsetter

GES DISC has developed a tool for subsetting the Aura HDF-EOS5 data files spatially, temporally, vertically, and by parameter. For Aura MLS, this subsetter provides spatial subseting of Aura/MLS Level-2 products and is available via GES DISC Web-based Hierarchial search and order Mechanism 'WHOM'. The original metadata and attributes are maintained during subsetting.

4.6 Other Tools for MLS Products

Below we list some other tools that support HDF/HDF-EOS and HDF5/HDF-EOS5 files and

can be used for Aura MLS Level-1B, 2 and 3 data products.

HDFView - A freeware Java-based application created by NCSA for browsing and editing contents of HDF4 and HDF5 and HDF-EOS & HDF-EOS5 data files. Objects are displayed in a tree listing. Data can be subsetted, and displayed in spreadsheets, as an image or saved to ASCII or XML format. Simple mathematical functions, linear plots, and histograms are supported. The latest version is modular in design and supports plug-ins.

IDL Based H5_BROWSER - The latest IDL version 6.1 supports HDF, HDF-EOS and HDF5. The H5_BROWSER function is a graphical tool for displaying and browsing the contents within an HDF5 file, and allows one to import these into the IDL environment for later use. IDL also includes wrappers for HDF5 functions so that one can write one's own custom code.

Command Line Tools

h5dump: a free tool from NCSA for dumping and subsetting contents of HDF5 files. The data may be output to ASCII or XML files; default is to the screen.

h5ls: a free tool from NCSA for listing the objects within an HDF5 file.

Format Converters

h4toh5: a free tool from NCSA for converting an old HDF4 file to the new HDF5 format.

h5toh4: a free tool from NCSA for converting HDF5 files back to the older HDF4 format.

Heconvert: a free EOS tool for converting an old HDF-EOS (based on HDF4.x) file to the new HDF-EOS5 format

hdfeos52netcdf: a tool for converting files in HDF-EOS5 to the netCDF file format.

4.7 Near-line Archive Data Mining (NADM)

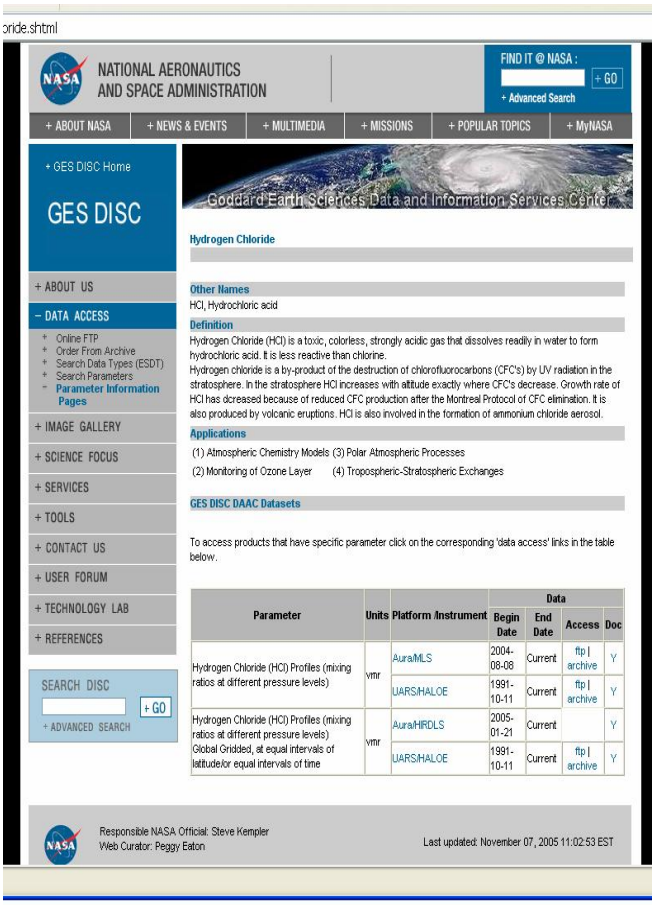
GES DISC gives registered users the capability to upload their data mining algorithms to test it on the data pool holdings at the GES DISC. No need to download the multi years of data sets for the temporal studies.

5. DATA ACESS

One of the main goals of the GES DISC is making the data easily accessible to the wider user community. All of the data sets archived at GES DISC are freely made available to the public and science user communities. These data sets may be accessed via several mechanisms including:

GES DISC Search and Order

A user friendly Web-based search and order system, with full-features of spatial & temporal search http://acdisc.gsfc.nasa.gov/data/



ACDISC Parameter Information (PIP) Interface

This Interface provides selection of specific atmospheric composition data from the parameter list which leads to the data pool and/or data archive site. (http://disc.gsfc.nasa.gov/PIP/)

EOS Data Gateway (EDG)

This interface provides access to all NASA data archive centers and NASA affiliated centers http://eos.nasa.gov/imswelcome/

Anonymous FTP Site (Data Pool)

A majority of the ACDISC data sets including MLS data products are available from the GES DISC anonymous FTP site (ftp://daac.gsfc.nasa.gov/data/) .

6. SUMMARY

Aura MLS is providing information on the vertical distribution of several key parameters for stratospheric and tropospheric chemistry and climate research. Extensive data validation activities (Froidevaux et al, 2006) are in progress to evaluate and improve algorithm by comparing products derived from in-situ observations.

The Aura MLS has improved capabilities over UARS MLS in providing many more trace gases day and night, with daily global coverage. It provides reliable measurements even in the presence of aerosol, cirrus, or polar stratospheric clouds that can degrade measurements based on UV, visible or thermal techniques.

Aura MLS provides data continuity to the ozone and other trace gases data record from UARS MLS and HALOE. MLS products will be used by the scientific community to monitor ozone, air quality and in quantifying the effects of atmospheric constituent's changes on the climate. MLS atmospheric products, including calibrated radiances are archived at the NASA Goddard Earth Sciences Data and Information Services Center (GES DISC) Distributed Active Archive Center (DAAC) and are freely available to the scientists and other data user communities. (http://acdisc.gsfc.nasa.gov/Aura/MLS/data_products.shtml

The Aura Data Support Team at the NASA Goddard DAAC has been providing science and data support to assist users in accessing and using the upper atmospheric composition data products. A number of tools for data access, subsetting, and visualization and data analysis have been developed at the NASA GES DISC (http://acidsc.gsfc.nasa.gov/tool.shml)

7. ACKNOWLEDGMENTS

This work is supported by the NASA Science Mission Directorate Earth-Sun System Division.

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* Updated and complete preprints of the above publications 'in press' are available at http://mls.jpl.nasa.gov/