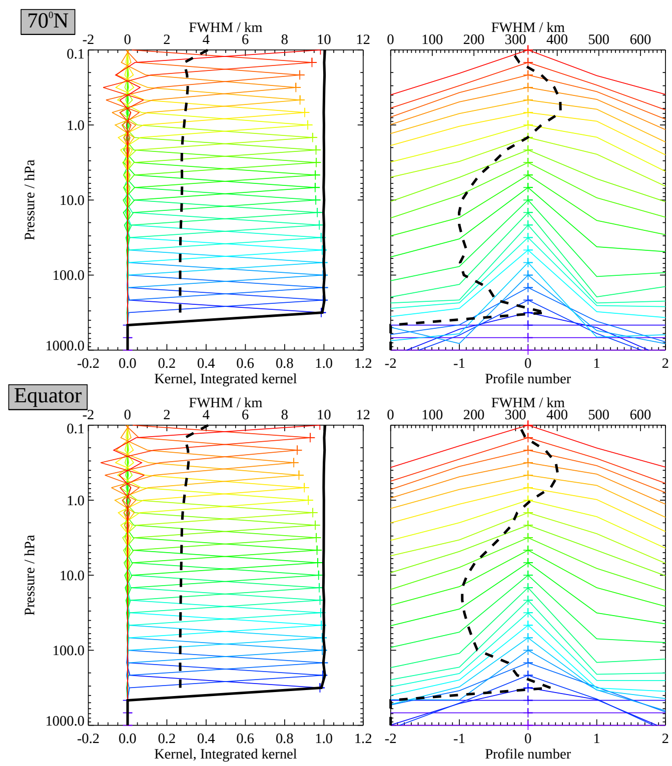
JPL D-48439

Earth Observing System (EOS)
Aura Microwave Limb Sounder (MLS)
Version 2.2 Level 2 near-real-time data user guide.



Alyn Lambert, Lucien Froidevaux, Michael J. Schwartz, William G. Read, Nathaniel J. Livesey, Paul A. Wagner, David T. Cuddy, Vincent S.Perun

Version 2.2x-NRT-1.0a
November 6, 2008

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California, 91109-8099

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Acknowledgment

This research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration.

1 Aura MLS Near-Real-Time Data Products

This document describes the production and data quality assessment of near-real-time (NRT) data from Aura MLS using a preliminary "reduced Level-2" algorithm data processing suite. The NRT retrievals use a fast linearized forward model resulting in computational resource requirements reduced dramatically compared to the standard product processing suite. Operational processing of the NRT temperature and ozone data started in February 2008 at the MLS SIPS. The data are distributed by the NASA Goddard Space Flight Center Earth Sciences Data and Information Servive Center (GSFC-DISC):

`http://daac.gsfc.nasa.gov`.

1.1 Aura MLS Instrument

The Aura Microwave Limb Sounder [Waters, 1993; Waters et al., 2006], an advanced successor to the MLS instrument on the Upper Atmosphere Research Satellite (UARS), is a limb sounding instrument which measures thermal emission at millimeter and sub-millimeter wavelengths using seven radiometers to cover five broad spectral regions. The radiometric and spectral performance of the MLS instrument is covered in detail by Jarnot et al. [2006] for the GHz radiometers and by Pickett [2006] for the THz radiometer.

The MLS line-of-sight is in the forward direction of the Aura spacecraft flight track. The Earth's limb is scanned from the surface to 90 km every 24.7 s giving 240 scans per orbit spaced at 1.5° intervals (165 km) with a total of ∼3500 vertical profiles per day and a nearly global latitude coverage from 82°S–82°N. The viewing geometry of the MLS instrument allows the innovative use of a 2-dimensional approach to the retrieval problem since the limb observations from successive scans overlap significantly which means that effects of line-of-sight gradients can be taken into account [Livesey and Read, 2000].

1.2 Aura MLS Retrievals

The MLS limb radiance measurements are inverted using an optimal estimation retrieval [Livesey et al., 2006] to yield atmospheric profiles of temperature, geopotential height, ozone, humidity and other trace gases. The MLS data are currently being produced as version 2.2 and uses GEOS-5 analyses as the a priori state for temperature. The validation of v2.2 products relevant to the planned NRT products is discussed in Froidevaux et al. [2008] for O_3, Schwartz et al. [2008] for temperature and Read et al. [2007] and Lambert et al. [2007] for H_2O. The version 2 data quality document is available from:

`http://mls.jpl.nasa.gov/data/v2-2_data_quality_document.pdf`.

However, the use of the standard MLS processing suite is not practical for processing a NRT data stream because of the large demands on computational resources and the inherent latency involved.

1.3 Motivation for providing Aura MLS NRT Data Products

In the following we highlight some recent studies concerning the use of Aura MLS standard product data in offline assimilation schemes.

- Jackson [2007] investigated the impact of assimilation of SBUV/2 and Aura MLS data into the Met Office Data Assimilation System for three experiments conducted for January-Feburary 2005 involving (i) a control where ozone was not assimilated, (ii) SBUV/2 ozone only, and (iii) SBUV/2 and MLS ozone. Compared to the experiment that included SBUV/2 data alone, addition of the higher vertical resolution Aura MLS data led to: reduction in the mean analysis error and standard deviation in the lower stratosphere, better representation of the northern hemisphere winter polar ozone depletion and better representation of southern hemisphere summertime low ozone events.

- Feng et al. [2007] used the ECMWF model to assimilate ozone from SBUV/2 and SCIAMACHY. Addition of the Aura MLS observations significantly improved the agreement with independent data from POAM III at southern high latitudes.

- Stajner et al. [2007] assimilated Aura MLS and OMI ozone data into the Goddard Earth Observing System version 4 (GEOS-4) data assimilation system. The derived tropospheric ozone columns reproduced the seasonal cycle and variability seen in independent ozone sonde data.

- A one-month assimilation of Aura MLS ozone data by the Global Data Assimilation Office (GMAO) GEOS-5 was reported in the JCSDA Quarterly (issue No.18,25 March 2007), showing that the assimilation using MLS data produced a realistic Antarctic ozone hole feature compared to the assimilation of the SBUV/2 data alone. Comparisons with independent South Pole ozone sondes revealed that the ozone profile shape in the lower stratosphere is reproduced more accurately in the MLS assimilation. In the tropics, the results showed that the assimilation including MLS data is in better agreement with independent HALOE and ozone sonde data compared to the assimilation of the SBUV/2 data alone.

The assimiliation of Aura MLS ozone data is expected to lead to:

- improvements in the temperature, radiation and heating fields internal to the models,
- improvements in the analysed ozone fields e.g. [Struthers et al., 2002; Wargan et al., 2005],
- improvements in air quality prediction through the estimation of tropospheric ozone e.g. [Struthers et al., 2002]
- more accurate regional and global forcecasts of surface UV radiation e.g. [Long et al., 1996],
- better description of stratospheric dynamics e.g. [Peuch et al., 2000],
- better planning and support of large coordinated atmospheric measurement campaigns e.g. [Newman et al., 2002]

2 Aura MLS NRT Retrievals

We have demonstrated the capability of providing Aura MLS NRT products for temperature and ozone by developing a set of preliminary "reduced Level-2" algorithms. These Level-2 NRT algorithms were developed using a simplified fast linearized forward model and subsequently are not as accurate as the retrievals that constitute the standard MLS products, but nevertheless the results are of scientific use and track the standard MLS products with reasonable fidelity as described in the following sections. At the lowest levels there are problems with the linear NRT ozone retrievals, notably at the lowest 215 hPa level and also at 147–100 hPa, at high latitudes and in the tropics. These are the regions where the second order forward model discussed in a later section will make significant improvements. It is expected that errors of up to 150 ppbv in ozone arising from a first-order approximation scheme will be corrected to within 50 ppbv by the second-order scheme.

2.1 Retrieval of NRT Temperature and Geopotential Height

2.1.1 Retrieval approach

The MLS NRT temperature product is a variant of the standard temperature product optimized for speed. A linear retrieval is employed using a restricted set of radiances and tables of precomputed Jacobians. Radiances used in the NRT temperature retrieval are from MLS band 1, a 25-channel filterbank centered on the 118-GHz oxygen line, and from bands 32 and 34, wideband channels on the wings of this line. These bands provide temperature information from the uppermost troposphere through the stratosphere. The NRT retrieval does not use radiances from band 22, which provide the standard retrieval with temperature information in the mesosphere and lower thermosphere but require a geomagnetic-field-dependent polarized forward model. Neither does it use radiances from the 240-GHz isotopic oxygen line (band 8), which provide upper-tropospheric-temperature information to the standard retrieval.

The NRT temperature also differs from the standard v2 product in the a priori used in the retrievals. The NRT retrieval uses CIRA86 climatology as its temperature a priori for all levels, while the standard v2 temperature retrieval uses GEOS-5 temperature as its a priori from the surface to 1 hPa and uses CIRA86 climatology only at smaller pressures.

The NRT temperature retrieval is 1-dimensional. The forward model for a given limb scan does not account for horizontal gradients in temperature. Standard MLS temperature is based upon a 2-D, "tomographic" retrieval where multiple limb scans are used to retrieve multiple profiles, including effects of horizontal gradients.

2.1.2 Comparison to v2.2 data

Biases between NRT and v2.2 temperature are generally less than 1 K between 68 hPa and 3.2 hPa. NRT temperature with respect to v2.2 has a low bias of 2.5 K at 1 hPa. This low bias drops to 1 K or less at 1.5 hPa at mid- and high-latitudes but extends to 1.5 K at 2.2 hPa in the tropics. At 100 hPa NRT temperature also has a low bias of $\sim$3 K in the tropics and and 1.5 K at high latitudes compared to v2.2. Correlation in the departures of NRT and v2.2 temperature from CIRA86 climatology are generally $\sim$0.8 or better between 178 hPa and 1 hPa. The exception is at 82 hPa and 68 hPa, where the correlation coefficient drops to 0.6. Scatter between NRT and v2.2 temperatures in the tropics and summer hemisphere is typically 1–1.5 K between 46 hPa and 6.8 hPa, increasing to 2.5 K at 1 hPa. Scatter above 40° latitude in the winter hemisphere increases to $\sim$5 K, which may in part be due to the 1-D nature of the NRT retrieval.

2.2 Retrieval of NRT Ozone

2.2.1 Retrieval approach

Ozone is measured in several microwave bands by Aura MLS. The standard product ozone retrievals use a non-linear simultaneous retrieval of O_3, temperature, CO, HNO_3, and SO_2 from several bands in the R3 240 GHz region. For the NRT ozone retrievals we also selected this same R3 240-GHz region, using band 7 (25-channel filter-bank spectrometer) and band 33 (4-channel wide-band) with a simultaneous retrieval of HNO_3 and SO_2, although these latter products are not distributed.

This first version of MLS NRT ozone retrievals includes some approximations in terms of the number of spectral channels used, and the fact that the full (non-linear) forward model is not used; an optical depth criterion is applied to limit the use of optically thicker channels. Several trials were made with optical depth cut-offs to select radiances from channels / heights which are not too non-linear.

2.2.2 Comparison to v2.2 data

These NRT retrieval approximations denoted above lead to a degraded product, compared to the v2.2 retrievals, although the ozone data set is of high enough quality between about 68 hPa and 0.2 hPa for general usage. Zonal mean differences between the NRT and v2.2 results are typically within 5 to 10% for pressures between 68 and 0.2 hPa. Comparisons between the two sets of stratospheric retrievals over many days reveal significant differences mostly for pressures of 100 hPa and larger. The largest differences occur at high latitudes during polar winter/spring; low values of ozone (less than 0.5 ppmv) are often significantly underestimated by the NRT retrievals near 100 to 150 hPa. Although NRT results at 100 hPa, outside the winter season, are sometimes close to the v2.2 results, they show enough oscillations in the tropics and during winter at high latitudes that it is probably best to ignore this pressure surface altogether. The use of these NRT data for deriving column ozone values, however, is less compromised by such oscillations, so the inclusion of column values down to 100 hPa may be sufficiently robust in most cases. Also, at high latitudes during winter, the NRT mixing ratios from 7 to 1 hPa can often be biased low by several tenths of a ppmv (more than 20%).

Finally, as a result of the reduced sensitivity (reduced number of channels), precisions in the NRT ozone data are poorer than for v2.2 in the lower stratosphere, often by a factor of two or more, especially so at high latitudes. We note an apparent improvement in precision for this preliminary product in the upper stratosphere compared to v2.2 which occurs because of incomplete propagation of errors from the temperature retrieval

In summary, it is felt that the NRT ozone values between 68 hPa and 0.2 hPa can generally be used for research (after applying the recommended data screening methods), with the possible inclusion of data down to 100 hPa for column ozone results.

2.3 NRT Data Quality Assessment

The Level-2 NRT processor generates the same three data quality metrics on a profile-by-profile basis (status, quality, convergence) that are provided for the standard MLS processing and hence are be available for immediate use in data assimilation schemes. Information on the use of the quality flags is contained in the MLS v2.2 data quality document:

`http://mls.jpl.nasa.gov/data/v2-2_data_quality_document.pdf`.

2.3.1 Temperature data screening

- NRT temperature profiles are only recommended for scientific use at pressure levels from 178 hPa to 1 hPa.
- Each temperature value has an associated precision. Values with associated precisions that are negative should not be used.
- Profiles with odd Status should not be used. Typical good NRT profiles have Status=68, indicating only that GEOS=5 a priori was not used. There is no cloud retrieval as part of the NRT processing so the cloud bits of Status (16="high cloud", 32="low cloud") are never set.
- Profiles with Quality < 0.6 or > 3 should not be used (extremely high values of Quality, corresponding to extremely low retrieval chi-square values, occur occasionally and should be considered to be pathological).
- Profiles with Convergence > 1.01 should not be used.

2.3.2 Ozone data screening

- NRT Ozone profiles are only recommended for scientific use at pressure levels 68–0.2 hPa, except for the calculation of ozone columns where the 100 hPa pressure level may be used.
- Each ozone value has an associated precision. Values with associated precisions that are negative should not be used.
- Profiles with odd Status should not be used.
- Typical good NRT profiles have Status=68, indicating only that GEOS-5 a priori temperature was not used. There is no cloud retrieval as part of the NRT processing so the cloud bits of Status (16="high cloud", 32="low cloud") are never set.

- Profiles with Quality < 1.2 or > 3 should not be used. Unlike for v2.2 ozone, no other Quality flag cut-off is provided for the upper troposphere, as the use of upper tropospheric NRT ozone values is not currently recommended.

- The Convergence flag is not useful for the NRT ozone retrievals and should be ignored.

2.4 NRT Data Processing Outline

The Aura MLS Science Data Processing System is described in detail by [Cuddy et al., 2006]. In the routine processing of the MLS data, the Level-1 and Level-2 processors (called Product Generation Executables, PGEs) are developed and tested in the Science Computing Facility (SCF). The SCF provides the services and resources to perform scientific algorithm development, science processing software development, scientific quality control, and scientific analysis. The final PGEs for a given MLS data version are delivered for use at the Science Investigator-led Processing System (SIPS). The SIPS provides a facility for producing the standard science data products through processing and reprocessing using the algorithms developed and tested in the SCF. This work leverages the infrastructure and experience within the MLS team built up from operating the SCF and SIPS and the associated interfaces to the Goddard Space Flight Center (GSFC) Earth Science Distributed Active Archive Center (GES-DAAC). The SIPS implementation of the NRT data processing system is presented in more detail by Mousessian and Vuu [2008].

GES-DISC interface to MLS SIPS The GES-DISC provides the appropriate spacecraft predictive ephemeris, orbit / attitude data and earth motion data. A new NRT Level-0 data product is constructed from Rate Buffered Data (RBD) by sub-dividing the orbit contacts (100 minutes) into files with a granularity of 15 minutes or less. Problems in the data stream involving time gaps, glitches and repeated data records are handled at this stage.

Modifications to the standard processing to provide a Level-1 NRT Processor In the routine processing the Level-1 processor accepts the 2-hr granule Level-0 input and the spacecraft ancilliary data, performs the radiometric callibration [Jarnot et al., 2006] and produces the Level-1B data product (calibrated radiances and associated uncertainties) for a single day. For the Level-1 NRT processor only selected GHz radiances needed for the NRT products need be calibrated. The granularity is determined directly by the Level-0 NRT granularity (15 minutes or less).

Modifications to the standard processing to provide a Level-2 NRT Processor In the routine processing the Level-2 processor accepts the Level-1B products and climatology data and produces the Level-2 geophysical data products [Livesey et al., 2006], diagnostic information and summary logs. The full-day is divided into 350 data chunks each consisting of about 10 profiles along the orbit track and each chunk is processed in parallel on a separate processor. For the Level-2 NRT processor the chunk size is determined by the Level-1B data granularity (15 minutes or less).

NRT Data Latency We define Level-2 the data latency to be the time from the satellite measurement to the production of the Level-2 output data files. Typically most of the data are produced within 5 hours and 50% are produced within 3 hours.

3 Aura MLS Near-Real-Time Plans

Work is in progress to improve the Aura MLS NRT data products and we plan to provide a new humidity product.

Improvements to the radiative transfer fast forward model The radiative transfer fast forward model is the major constraint on the speed of the MLS NRT processor and the accuracy of the retrievals. The optically thin radiances are nearly linear in terms of the species concentrations, but a more accurate representation that holds for larger optical depths is a second-order Taylor series given in Equation 1,

$$
\begin{aligned}
I &= \overset{\star}{I} + \sum_l \overset{\star}{K}_j \left(x_l - \overset{\star}{x}_l\right) \\
&\quad + \frac{1}{2} \sum_l \sum_k \overset{\star}{L}_{jk} \left(x_l - \overset{\star}{x}_l\right) \left(x_k - \overset{\star}{x}_k\right), \\
\overset{\star}{K}_l &= \frac{\partial \overset{\star}{I}_i}{\partial x_l}, \\
\text{and,} & \\
\overset{\star}{L}_{lk} &= \frac{\partial^2 \overset{\star}{I}}{\partial x_l \partial x_k}, \qquad (1)
\end{aligned}
$$

where I is the calculated radiance, $\overset{\star}{I}$ is the radiance calculated at the linearization point, $\overset{\star}{x}_l$ is the extended state vector of species concentrations, temperature, and tangent pressure, $\overset{\star}{K}_l$ are the first-order derivatives of the forward model radiances with respect to the state vector, and $\overset{\star}{L}_{lk}$ are the second-order derivatives.

In the current version of the NRT data processing the forward model uses a first-order correction scheme (i.e. linear) stored as tabulated coefficients ($\overset{\star}{I}$ and $\overset{\star}{K}_l$) as a function of time (monthly bins) and latitude (7.5 degree bins).

We are in the process of developing a second-order correction scheme, also to be stored as tabulated coefficients ($\overset{\star}{L}_{lk}$). The use of the second-order coefficients in the forward model will produce more accurate radiances, but at relatively low cost in terms of execution time. Preliminary work on a second-order scheme was carried out for UARS MLS, but was not implemented in the operational code (see appendix G *The UARS MLS Radiance Model* of Read et al. [2003]).

In order to incorporate the second-order forward model the Level-2 processor requires significant coding changes in addition to changes to the Level-2 configuration file [Livesey et al., 2006] which is effectively a high-level language used to specify all aspects of the retrieval.

3.1 Advanced Aura MLS NRT Retrievals

- Provide a near-real-time end-to-end processing capability for Aura MLS measurements of ozone, temperature and humidity.
- Develop, implement and test the NRT processor package for delivery to Joint Center for Satellite Data Assimilation (JCSDA) partners.

Schedule for releasing advanced NRT data products

- Advanced NRT data products are expected to be released in the following cycle for ozone (Summer 2009), temperature (Winter 2009) and humidity (Summer 2010).
  - Phase I: Algorithm development and validation
    - Improve the NRT fast forward model accuracy

    * Arrange and test new NRT data feeds and interfaces
- Phase II: Create and test the configuration for the NRT ozone retrieval
    * Produce a one month data set, validate and deliver
    * Access the data quality control metrics
    * Produce a one year test data set, validate and deliver
    * Provide a data quality description document
    * Package and release the end-to-end NRT processor
    * Upgrade the MLS SIPS NRT operational processor
- Repeat Phase II for the temperature and humidity retrievals

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