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Earth Observing System (EOS)
Aura Microwave Limb Sounder (MLS)

Version 4 Level-2 near-real-time data user guide.

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1 Aura MLS Near-Real-Time Data Products

This document describes the production and data quality assessment of near-real-time (NRT) data from the Aura MLS instrument using modified Level-2 algorithms. 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. Consequently, the NRT retrievals have been adapted to reduce dramatically the computational resource requirements compared to the standard product processing suite. The NRT retrievals produce a subset of MLS products (T, O_3, CO, HNO_3, SO_2, H_2O, N_2O) using a reduced selection of the available MLS Level-1 radiances, coupled with lower fidelity forward model approximations which also neglect line-of-sight temperature and concentration gradients. As a result, the faster processing algorithms result in a degradation in the NRT data quality compared to the standard products. Typically most of the Level-2 NRT data are produced within 5 hours and over 94% are produced within 3 hours of the satellite observations.

Operational processing of the NRT products is carried out in an independent production stream at the MLS Science Investigator-led Processing System (SIPS). The data are distributed by the NASA Goddard Space Flight Center Earth Sciences Data and Information Service Center (GSFC-DISC) and are available through a subscription service:

`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.

1.2 Aura MLS Standard Product 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 4.2 and use GEOS-5 analyses as the a priori state for temperature. The validation of the MLS Level-2 standard products corresponding to the NRT products is discussed in the references given in the v4.2 standard product data quality document available from:

`http://mls.jpl.nasa.gov/data/v4-2_data_quality_document.pdf`.

2 Aura MLS NRT Retrievals

We have expanded our existing capability to provide Aura MLS products in near real time by developing an improved Level-2 v4.2-NRT algorithm. We produce temperature, ozone, carbon monoxide, water vapor, nitrous oxide, nitric acid and sulfur dioxide in the near real time data stream. These Level-2 NRT algorithms employ a simplified forward model and subsequently are not as accurate as the retrievals that constitute the standard MLS products. However, the results are of scientific use and track the standard MLS products with reasonable fidelity as described in the following sections.

A primary objective of the updated v4.2-NRT algorithm is to use radiances covering the 118-GHz oxygen line center to extend the NRT temperature retrieval through the mesophere. Interaction of oxygen with the geomagnetic field necessitates use of a computationally-expensive polarized forward model for these radiances, and the resulting slower temperature retrieval must be run in parallel with the constituent retrieval to meet the desired NRT latency goals.

2.1 Retrieval approach

Standard MLS retrievals are based upon a 2-D, "tomographic" retrieval where multiple limb scans are used to retrieve multiple profiles, including effects of horizontal gradients. All the NRT retrievals are one-dimensional and the forward model for a given limb scan does not account for horizontal gradients along the line-of-sight, i.e. each retrieved profile uses only radiances from the nearest single limb scan and retrieves a single profile, with no attempt to model along-track gradients. The NRT retrievals include some approximations in terms of the number of spectral channels used and e.g., an optical depth criterion is applied to limit the use of optically thicker channels.

Note that (a) the NRT HNO_3 profile data is a hybrid product of the 190-GHz ($p \leq 46$ hPa) and 240-GHz ($p \geq 68$ hPa) retrievals and (b) the NRT SO_2 profile data is obtained from the 240-GHz retrievals.

2.1.1 118-GHz Region

Temperature and geopotential height are retrieved from the 118-GHz region from four radiance bands (bands 1, 21, 32 and 34). 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 band 22, a high-resolution-spectrometer (Digital Auto-Correlator Spectrometer, DACS). Bands 32 and 34 are wide-band channels on the wings of oxygen line. Taken together, these bands provide temperature information from the uppermost troposphere through the stratopause and into the mesosphere and lower thermosphere. Band 22 radiances (which provide temperature information above the stratopause) are a new addition to the v4 NRT processing and required the implementation of a geomagnetic-field-dependent polarized forward model similar to that used for the standard temperature product.

The v4 NRT retrieval does not use radiances from the 240-GHz isotopic oxygen line (band 8), which provide upper-tropospheric-temperature information to the standard retrieval, because these require the addition of cloud screening which is not implemented in the NRT processor.

The NRT temperature also differs from the standard v4.2 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 v4.2 temperature retrieval uses GEOS-5 temperature as its a priori from the surface to 1 hPa and uses CIRA86 climatology only at smaller pressures.

2.1.2 240-GHz Region

SO_2, HNO_3, O_3, and CO are retrieved jointly in the 240-GHz region from a combination of two 25-channel filter-bank spectrometers (MLS radiance bands 7 and 9) and a 4-channel wide-band filter (MLS band 33).

2.1.3 190-GHz Region

H_2O, N_2O, HNO_3, and SO_2 are retrieved jointly in the 190-GHz region from a combination of three 25-channel filter-bank spectrometers (MLS radiance bands 2, 3, and 4).

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 available for immediate use in data assimilation schemes. Information on the HDF5-EOS data file structure and access to the quality flags is contained in the MLS v4.2 standard product data quality document:

`http://mls.jpl.nasa.gov/data/v4-2_data_quality_document.pdf`.

In the sections below we indicate the recommended screening for the NRT data products. The NRT data are processed and distributed in overlapping granules (chunks) of typical length 46 profiles. In Section 4.1 we outline a procedure for the removal of redundant data from the chunk overlaps.

3.1 Temperature data screening

Usable pressure range. The NRT Temperature product uses additional radiances from the high-resolution spectrometer on the 118-GHz line center and a polarized forward model to extend retrievals through the mesosphere. NRT temperature profiles may be scientifically useful at pressure levels from 215 hPa to 0.001 hPa.

Precision. Each value has an associated precision. Values with associated precisions that are negative should not be used.

Status flag. Profiles with odd Status should not be used. Typical good NRT profiles always have Status=68, indicating that the temperature a priori uses the CIRA climatology rather than GEOS-5 temperature. 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.

Quality. Profiles with Quality < 0.5 or > 3.0 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). This Quality threshold flags ∼5% of profiles as bad, predominantly at the edge of the polar winter vortex, where there are large along-track temperature gradients. At some levels, near the vortex edge, there are large (greater than ±30 K) differences between retrievals from ascending and descending halves of the orbit.

Convergence. Profiles with Convergence $>$ 1.05 should not be used. This threshold rejects only ∼0.5% of profiles, most of which are already rejected due to odd status (typically too few radiances).

Vertical resolution. From 215 hPa – 147 hPa, retrievals have as much contribution from the adjacent level above as from the eponymous level. The retrieval vertical averaging kernel FWHM is ∼5 km at 215 hPa, improving to 4 km at 147–100 hPa and to 3 km in the lower stratosphere. At 10 hPa, the vertical resolution is 4 km and it degrades to 8 km at 1.47 hPa and 10 km at 1 hPa.

Horizontal resolution. Horizontal resolution is 165 km, degrading to 195 km at the highest and lowest recommended levels.

Comments/Artifacts. NRT temperature is biased with respect to the v4.2 standard product, with the biases approaching ± 10 K in some places and changing signs between the ascending portion and descending portions of the orbit. This is believed to be an artifact due to the use of 1-D retrievals for the NRT product. Biases are largest on the edge of the winter polar vortex and oscillate with height. Since the v4 NRT retrieval uses radiances from the high resolution band 22 118-GHz DACS, ignored in prior NRT versions, the retrieval has consequently been extended to pressures less than 1 hPa. In initial tests, v4.2-NRT and the v4.2 production mesospheric temperatures have mean differences of typically 2.5 K or less in magnitude, with 1-sigma scatter about these means increasing from ∼3 K at 1 hPa to ∼6 K at 0.01 hPa. The retrieval is limited in the upper-troposphere by its neglect of the isotopic $O^{18}O$ channels radiances in the 234 GHz region (band 8).

3.2 Ozone data screening

Usable pressure range. NRT Ozone profiles are only recommended for scientific use at pressure levels from 261 hPa to 0.1 hPa.

Precision. Each value has an associated precision. Values with associated precisions that are negative (which indicates too strong an influence from the a priori) should not be used.

Status flag. Profiles with odd Status (typically less than 2 to 3% of profiles) should not be used. Typical good NRT profiles have Status=68, indicating that the temperature a priori uses the CIRA climatology rather than GEOS-5 temperature. 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. Retrievals for which there were not enough radiances (Status 325) are also typically poorly converged.

Quality. Profiles with Quality $<$ 0.2 should not be used. This typically removes less than 1% of profiles, but this screening probably will have very little impact on scientific results and is not strongly recommended.

Convergence. Profiles with Convergence $>$ 1.2 should not be used. This typically removes less than 0.5 to 1% of profiles. These profiles tend to have slightly poorer agreement with values from the v4.2 production retrieval than do those with lower convergence. However, removal of these profiles likely has very little impact on scientific results and is not strongly recommended.

Vertical resolution. The vertical resolution of the retrieval (averaging kernel FWHM) is 2.5–3 km for p $>$6.8 hPa and 3–4 km for the pressure range 6.8 hPa $<$ p $<$ 0.1 hPa.

Horizontal resolution. The horizontal resolution is 165–215 km.

Comments/Artifacts. In most of the stratospheric range, namely from about 68 to 1 hPa, typical biases between the NRT ozone and the v4.2 standard product amount to less than a few percent, with equally low scatter (standard deviation) in the differences. There are larger biases and scatter (typically up to 20-30%) for the lower mesosphere and into the upper mesosphere (the latter is not well measured, given the reduced choice of frequency channels for the NRT software); users interested in the lower mesosphere are advised to use MLS NRT values there with some caution.

3.3 Carbon monoxide data screening

Usable pressure range. v4.2-NRT Carbon monoxide profiles are only recommended for scientific use at pressure levels from 215 hPa to 0.1 hPa.

Precision. Each value has an associated precision. Values with associated precisions that are negative (which indicates too strong an influence from the a priori) should not be used.

Status flag. Profiles with odd Status (typically less than 2 to 3% of profiles) should not be used. Typical good NRT profiles have Status=68, indicating that the temperature a priori uses the CIRA climatology rather than GEOS-5 temperature. 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. Retrievals for which there were not enough radiances (Status 325) are also typically poorly converged.

Quality. Profiles with Quality $<$ 0.2 should not be used. This typically removes less than 1% of profiles, but this screening probably will have very little impact on scientific results and is not strongly recommended.

Convergence. Profiles with Convergence $>$ 1.2 should not be used. This typically removes less than 0.5 to 1% of profiles; these profiles tend to have slightly poorer agreement with values from the v4.2 production retrieval than do those with lower convergence. However, removal of these profiles likely has very little impact on scientific results and is not strongly recommended.

Vertical resolution. The vertical resolution of the retrieval (averaging kernel FWHM) is expected to be very similar to that of the v4.2 NRT product ($\sim$5.5 km at 215 hPa and 5 km at 100 hPa).

Horizontal resolution. The horizontal resolution is 235 km at 215 hPa and 165 km at 100 hPa.

Comments/Artifacts. Vertical averaging kernel at some levels in the UTLS have slightly negative responses to CO two levels below their nominal response levels. For example, extremely high CO mixing ratios at 215 hPa from convectively lofted fire plumes in 2009 and 2017 led to negative artifacts at 100 hPa, and a similar anomalous negative response at 68 hPa resulted from extremely elevated values at 147 hPa.

3.4 Water vapor data screening

Usable pressure range. v4.2-NRT water vapor profiles are only recommended for scientific use at pressure levels from 147 hPa to 1 hPa.

Precision. Each value has an associated precision. Values with associated precisions that are negative (which indicates too strong an influence from the a priori) should not be used.

Status flag. Profiles with odd Status should not be used. Typical good NRT profiles have Status=68, indicating that the temperature a priori uses the CIRA climatology rather than GEOS-5 temperature. 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.

Quality. Profiles with Quality ≤ 0 should not be used.

Convergence. Profiles with Convergence > 3.0 should not be used.

Vertical resolution. The vertical resolution of the retrieval (averaging kernel FWHM) is 2.1–3.5 km.

Horizontal resolution. The horizontal resolution is 165–170 km.

Comments/Artifacts. The 147 hPa H_2O is too dry for low values (higher latitudes) and possibly too moist for high values (lower latitudes). The morphology of the data is acceptable. The other levels at 121 hPa and smaller pressures agree well with the standard product v4.2 data.

3.5 Nitrous oxide data screening

Usable pressure range. v4.2-NRT nitrous oxide profiles are only recommended for scientific use at pressure levels from 100 hPa to 1 hPa.

Precision. Each value has an associated precision. Values with associated precisions that are negative (which indicates too strong an influence from the a priori) should not be used.

Status flag. Profiles with odd Status should not be used. Typical good NRT profiles have Status=68, indicating that the temperature a priori uses the CIRA climatology rather than GEOS-5 temperature. 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.

Quality. Profiles with Quality < 0.2 should not be used.

Convergence. Profiles with Convergence > 3.0 should not be used.

Vertical resolution The vertical resolution of the retrieval (averaging kernel FWHM) is 4.7–8.5 km

Horizontal resolution The horizontal resolution is 165–320 km.

Comments/Artifacts. On the 68-hPa surface N_2O NRT values in the tropics are 20–25% smaller than the standard v4.2 product.

3.6 Nitric acid data screening

Usable pressure range. v4.2-NRT nitric acid profiles are only recommended for scientific use at pressure levels from 100 hPa to 1.5 hPa.

Precision. Each value has an associated precision. Values with associated precisions that are negative (which indicates too strong an influence from the a priori) should not be used.

Status flag. Profiles with odd Status should not be used. Typical good NRT profiles have Status=68, indicating that the temperature a priori uses the CIRA climatology rather than GEOS-5 temperature. 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.

Quality. For pressure levels $\geq$ 68 hPa, profiles with Quality $<$ 0.2 should not be used. For pressure levels $\leq$ 46 hPa, the Quality screening is not useful and the data should be used with caution.

Convergence. For pressure levels $\geq$ 68 hPa, profiles with Convergence $>$ 1.2 should not be used. For pressure levels $\leq$ 46 hPa, the Convergence screening is not useful and the data should be used with caution.

Vertical resolution. The vertical resolution of the retrieval (averaging kernel FWHM) is 3.0–5.0 km.

Horizontal resolution. The horizontal resolution is 165–220 km.

Comments/Artifacts. The NRT HNO_3 profile data is a hybrid product of the 190-GHz ($p \leq$ 46 hPa) and 240-GHz ($p \geq$ 68 hPa) retrievals.

3.7 Sulfur dioxide data screening

Usable pressure range. v4.2-NRT sulfur dioxide profiles are only recommended for scientific use at pressure levels from 215 hPa to 10 hPa.

Precision. Each value has an associated precision. Values with associated precisions that are negative (which indicates too strong an influence from the a priori) can be used for volcanic injection detection, but the values will be underestimated compared to the standard product SO_2.

Status flag. Profiles with odd Status should not be used. Typical good NRT profiles have Status=68, indicating that the temperature a priori uses the CIRA climatology rather than GEOS-5 temperature. 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.

Quality. Profiles with Quality ≤ 0 should not be used.

Convergence. Profiles with Convergence > 1.8 should not be used.

Vertical resolution. The vertical resolution of the retrieval (averaging kernel FWHM) is 3.0–3.7 km.

Horizontal resolution. The horizontal resolution is 165 km.

Comments/Artifacts. Values with associated negative uncertainties (meaning too much a priori influence) can be used for detection of volcanoes or other high events; however the retrieved value will be too low because the retrieval is biased towards its zero a priori.

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).

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 ancillary 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 the NRT 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 94% are produced within 3 hours. MLS NRT data are distributed in granules (chunks) of typical length 46 profiles.

4.1 Recomendation for the treatment of MLS NRT data overlaps

Chunk overlaps (redundant data records) are required so that our NRT processing system produces reliable calibrated radiances and data retrievals across the chunk boundaries. Profiles in the chunk overlaps can be identified from the time stamps in each file. Figure 1 shows an example where the chunk (granule) length is 46 profiles.

The data quality at the beginning and end of a chunk is known to be worse than within the chunk. Therefore, we recommend the following procedure to remove the poorer quality profiles and to prevent using two profiles with the same time stamp:

1 Discard the first two profiles and the last three profiles of every chunk as the data quality is known to be poorer at these locations (shaded red in Figure 1).

2 After discarding these profiles there is little difference in the data quality in the remaining duplicate profiles (shaded blue in Figure 1) in the overlap region, however it may be expedient to use the profiles in the first chunk (39-43) rather than wait to process the second chunk.

3 Poor quality profiles 1-2 in the second chunk (shaded red in Figure 1) will be discarded since the higher quality profiles 37-38 from the first chunk (shaded green in Figure 1) will have been used.

4 Higher quality profiles 8-10 (shaded green) in the second chunk will be used in place of the discarded profiles 45-46 in the first chunk (shaded red in Figure 1).

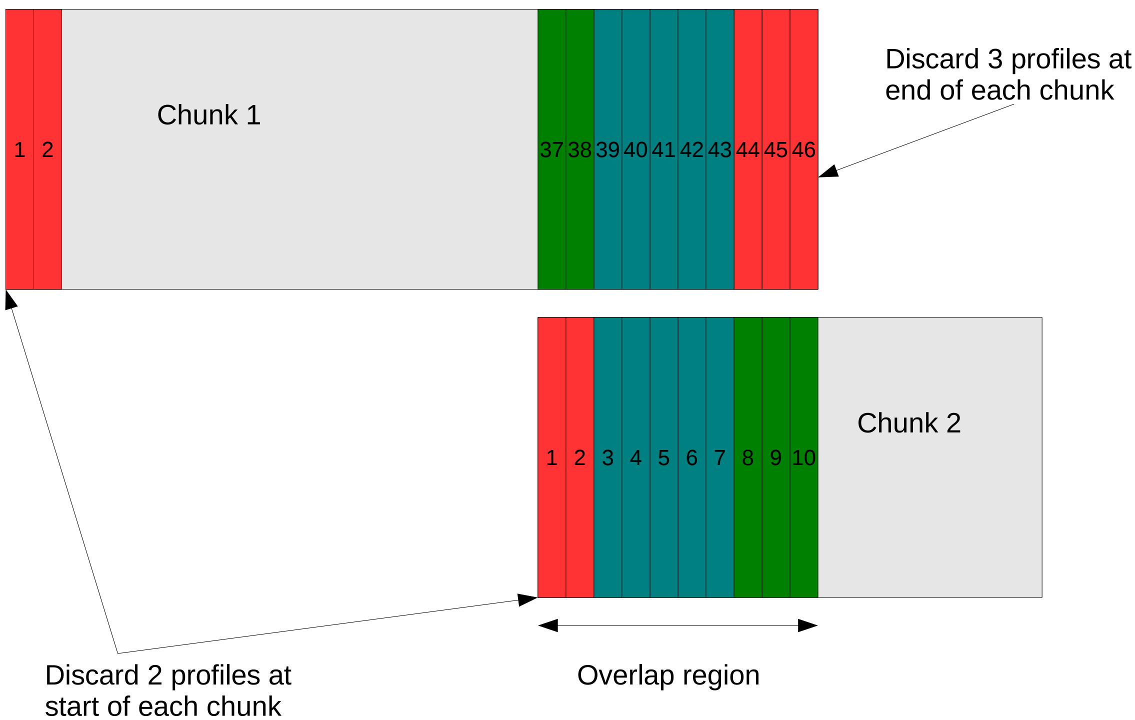

Figure 1: Treatment of MLS NRT data overlaps.

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