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

**Version 5 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) v05.01-NRT data from the Aura MLS instrument. 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. The application of machine learning techniques to predict the NRT products dramatically reduces the computational resource requirements compared to the standard product processing suite. The NRT algorithm produces a subset of MLS products (T, O₃, CO, H₂O, N₂O, HNO₃, SO₂) based on predictions from individually trained feedforward artificial neural networks (ANN). Typically over 94% of the Level-2 NRT data are produced within 3 hours and most data are produced within 5 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 through a subscription service by the NASA Goddard Earth Sciences Data and Information Services Center (GES-DISC) :

<https://disc.gsfc.nasa.gov>

and are also available from the Land, Atmosphere Near real-time Capability for EOS (LANCE) website

<https://earthdata.nasa.gov/earth-observation-data/near-real-time/download-nrt-data/mls-nrt>

Orbit track visualizations of MLS NRT data are available for the following products and pressure levels : CO at 215 hPa, SO₂ at 147 hPa and H₂O, O₃, N₂O, and HNO₃ at 46 hPa on the NASA WorldView website :

<https://worldview.earthdata.nasa.gov>

1.1 Aura MLS Instrument

The Aura Microwave Limb Sounder [Waters, 1993; Waters et al., 2006] 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 5.01 and use GEOS-5

analyses as the a priori state for temperature. The data file format, characteristics, screening rules, and validation of the MLS Level-2 standard products corresponding to the NRT products is discussed in the v5.0 standard product data quality document (and references therein) available from:

https://mls.jpl.nasa.gov/data/v5-0_data_quality_document.pdf

2 Aura MLS NRT Retrievals

The primary improvement in the v05.01-NRT algorithm is the use of ANNs to predict the profiles for all NRT products. The predictions for each NRT product are based on 18 separate ANNs for each 10-degree latitude bin from -90° to 90° . The networks were trained on 75% of the valid v5 MLS standard product retrievals between January 2005 and April 2022 and their associated, nearest radiance profiles. To avoid overfitting, 20% of valid v5 data was used internally as a validation data set. The ANN performance was evaluated using an independent test data set, which comprises the remaining 5% of profiles. As the MLS v5 standard products are used as “truth” in the training, the best-case output of the ANN is a computationally-inexpensive, high-fidelity preview of the v5 profiles.

A comprehensive description of the methodology, individual settings, and performance evaluation of the models is given in:

Werner et al. (2022), Applying machine learning to improve the near-real-time products of the Aura Microwave Limb Sounder, Atmos. Meas. Tech., to be submitted

3 NRT Data Quality Assessment

Each profile value has an associated precision, although these are not produced for individual profiles by the ANNs. Rather, the reported values are the root sum square of (i) the typical level 2 precisions for the given pressure level taken from the training data and (ii) the root-mean-square deviation between MLS v5 standard products and the predictions for the independent test data set. Data values whose associated precisions are set negative should not be used. Negative precisions are assigned to values outside the valid pressure range, profiles in overlap regions (see Section 4.1), as well as those containing invalid radiances.

The precision values are also used to represent the data quality. The quality check assures that predictions at each pressure level are within a predefined confidence range. This range is derived from the minimum and maximum of the v5 MLS retrievals at each level (from the full data set) and the difference between the maximum and minimum value. If a profile contains a prediction, at any level, that is smaller than the minimum negative difference or larger than the maximum positive difference all the associated precisions are set to be negative. Other quality metrics like status, quality, and convergence are not used.

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. NRT temperature profiles may be scientifically useful at pressure levels from 261 hPa to 0.001 hPa.

Precision. Only use values with positive precisions.

Vertical resolution. Since the neural network models have been trained on the v5 level 2 temperature standard product retrievals, the vertical and horizontal resolutions are comparable to the standard product.

From 261 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. Correlation coefficients between the v5 level 2 temperature retrievals and NRT predictions are larger than 0.95 within the valid pressure range. For pressure levels between 146 and 0.3 hPa the 1st/99th percentile of the difference between the two data sets is smaller than 5 K. No significant NRT temperature biases are observed compared to the standard product at any pressure level.

3.2 Ozone data screening

Usable pressure range. NRT O₃ profiles are only recommended for scientific use at pressure levels from 316 hPa to 0.046 hPa.

Precision. Only use values with positive precisions.

Vertical resolution. The vertical resolution of the L2 v5 retrieval (averaging kernel FWHM) is 2.5–3 km for $p > 6.8$ hPa and 3–4 km for the pressure range $6.8 \text{ hPa} < p < 0.1 \text{ hPa}$.

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

Comments/Artifacts. Correlation coefficients between the v5 level 2 O₃ retrievals and NRT predictions are larger than 0.82 within the valid pressure range (> 0.92 between 316 and 6.8 hPa). For pressure levels between 316 and 0.1 hPa the median difference between the two data sets is smaller than 1%.

3.3 Carbon monoxide data screening

Usable pressure range. NRT CO profiles are only recommended for scientific use at pressure levels from 215 hPa to 0.0046 hPa.

Precision. Only use values with positive precisions.

Vertical resolution. The vertical resolution of the L2 v5 retrieval (averaging kernel FWHM) is ~ 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. Correlation coefficients between the v5 level 2 CO retrievals and NRT predictions are larger than 0.7 in the UTLS and > 0.96 for pressures < 1 hPa. For pressure levels between ~ 21.5 and 3.2 hPa the correlations are < 0.6 . Here, both the v5 level 2 retrievals and the ANN predictions are just noise. For all recommended pressure levels the median difference between the two data sets is smaller than 20%.

3.4 Water vapor data screening

Usable pressure range. NRT H₂O profiles are only recommended for scientific use at pressure levels from 316 hPa to 0.002 hPa.

Precision. Only use values with positive precisions.

Vertical resolution. The vertical resolution of the L2 v5 retrieval (averaging kernel FWHM) is 2.1–3.5 km.

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

Comments/Artifacts. Correlation coefficients between the v5 level 2 H₂O retrievals and NRT predictions are larger than 0.65 within the recommended pressure range. At almost all levels the median difference between the two data sets is smaller than 5%.

3.5 Nitrous oxide data screening

Usable pressure range. NRT N₂O profiles are only recommended for scientific use at pressure levels from 68 hPa to 0.46 hPa.

Precision. Only use values with positive precisions.

Vertical resolution The vertical resolution of the L2 v5 retrieval (averaging kernel FWHM) is 4.7–8.5 km

Horizontal resolution The horizontal resolution is 165–320 km.

Comments/Artifacts. Correlation coefficients between the v5 level 2 N₂O retrievals and NRT predictions are larger than 0.92 for pressures > 3.2 hPa. For lower pressure levels both the v5 level 2 retrievals and the ANN predictions are just noise. The median difference between the two data sets is smaller than 10% for the entire recommended pressure range.

3.6 Nitric acid data screening

Usable pressure range. NRT HNO₃ profiles are only recommended for scientific use at pressure levels from 215 hPa to 1.5 hPa.

Precision. Only use values with positive precisions.

Vertical resolution. The vertical resolution of the L2 v5 retrieval (averaging kernel FWHM) is 3.0–5.0 km.

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

Comments/Artifacts. Correlation coefficients between the v5 level 2 HNO₃ retrievals and NRT predictions are larger than 0.75 for pressures levels larger than 10 hPa. For pressures levels below < 3.2 hPa both the v5 level 2 retrievals and the ANN predictions are just noise. The median difference between the two data sets is smaller than 10% for almost the entire recommended pressure range.

3.7 Sulfur dioxide data screening

Usable pressure range. NRT SO₂ profiles are only recommended for scientific use at pressure levels from 215 hPa to 10 hPa.

Precision. Only use values with positive precisions.

Vertical resolution. The vertical resolution of the L2 v5 retrieval (averaging kernel FWHM) is 3.0–3.7 km.

Horizontal resolution. The horizontal resolution is 165 km.

Comments/Artifacts. Outside of volcanic plumes, both the v5 level 2 retrievals and the ANN predictions are basically just noise. The ANNs have been trained on major volcanic eruptions throughout the MLS mission and correlation coefficients between the v5 level 2 SO₂ retrievals and NRT predictions are > 0.5 throughout the recommended pressure range. The median difference between the two data sets is smaller than 20%.

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 NASA Goddard Earth Sciences Data and Information Services Center (GES-DISC).

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 calibration [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 MLS standard processing the Level-2 processor accepts the Level-1B products 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 MLS Level-2 NRT processor the chunk size is determined by the Level-1B NRT 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 Recommendation concerning 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.

- 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.
- 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).

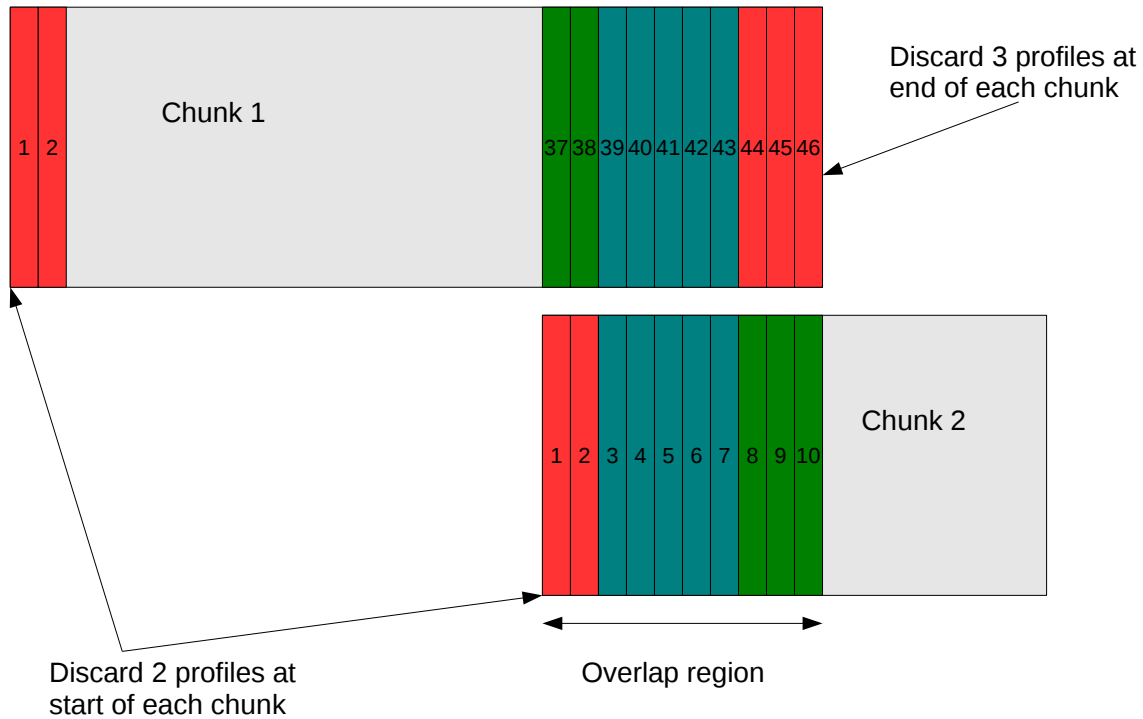


Figure 1: Treatment of MLS NRT data overlaps.

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