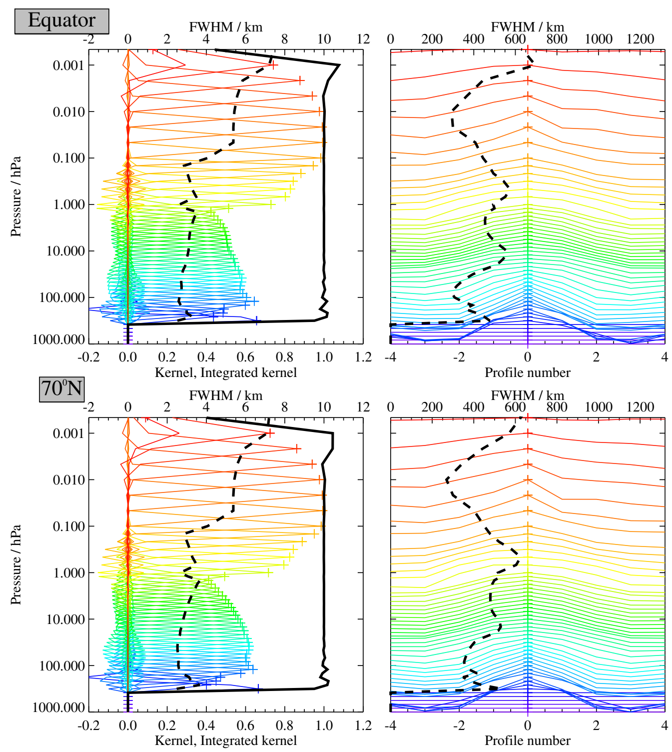
JPL D-105336 Rev. B

Earth Observing System (EOS)

Aura Microwave Limb Sounder (MLS)

Version 5.0x Level 2 and 3 data quality and description document.



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Navigating this document

Clicking on “Help” takes you back to this page.

An overview of the information in this document is given on the next page. You can return to it by clicking on the “Overview” tab in the navigation bar.

First-time users of MLS data are advised to read Chapter 1 first. The discussion includes a table summarizing key aspects of each MLS product. This table can be accessed from anywhere in the document by clicking on the “Table” tab in the navigation bar.

Chapter 3 describes each of the MLS data products individually. You can use the navigation bar to skip immediately to any of the product-specific sections.

Each section includes

- A set of rules for screening out data not recommended for scientific use.
- A table summarizing the precision, accuracy, resolution, etc., for each product.

Clicking on the product name in the navigation bar takes you to the beginning of that section; clicking on the “S” and “T” symbols takes you directly to the screening rules and summary table, respectively, for that product.

Acknowledgment

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Where to find answers to key questions

This document serves two purposes. Firstly, to summarize the quality of version 5.0 Aura MLS Level 2 and Level 3 data. Secondly, to convey important information to the scientific community on how to read and interpret the data.

The MLS science team strongly encourages users of MLS data to thoroughly read this document. Chapter 1 describes essential general information for all users. Chapter 2 is considered background material that may be of interest to data users. Chapter 3 discusses individual MLS data products in detail.

For convenience, this page provides information on how to quickly ascertain answers to anticipated key questions.

Where do I get v5.0*x* MLS data?

All the MLS Level 2 data described here can be obtained from the NASA Goddard Space Flight Center Earth Science Data and Information Services Center (GES-DISC, see `https://disc.gsfc.nasa.gov/`).

What format are MLS data files in?

MLS Level 2 data are in HDF-EOS version 5 format (section 1.5, page 4). Level 3 data are in netCDF 4 (section 4.2, page 169).

Which MLS data points should be avoided? How much should I trust the remainder?

These issues are described in section 1.6 (starting on page 6), and on a product by product basis in chapter 3. The key rules are:

- Only data within the appropriate pressure range (described product by product in chapter 3) are to be used.
- Always consider the precision of the data, as reported in the `L2gpPrecision` field.
- Do not use any data points where the precision is zero or a negative number. This indicates poor information yield from MLS.
- Do not use data for any profile where the field `Status` is an odd number.
- Data for profiles where the `Status` field is a non-zero even number should be approached with caution. See Section 1.6 on page 6, and the product by product description in Chapter 3 for details on how to interpret the `Status` field.
- Do not use any data for profiles where the `Quality` field is *smaller* than the threshold given in the section of Chapter 3 describing your product of interest.
- Do not use any data for profiles where the `Convergence` field is *larger* than the threshold given in the section of Chapter 3 describing your product of interest.
- Some products require additional screening to remove biases or outliers (see chapter 3).
- Chapter 3 also provides information on the accuracy of each product.
- Data users are strongly encouraged to contact the MLS science team to discuss their anticipated usage of the data, and are always welcome to ask further data quality questions.

Why do some species abundances show negative values, and how do I interpret these?

Some of the MLS measurements have a poor signal to noise ratio for individual profiles. Radiance noise can naturally lead to some negative values for these species. It is critical to consider such values in scientific study. Any analysis that involves taking some form of average will exhibit a high bias if the points with negative mixing ratios are ignored.

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Document revision history

Version 5.0x-1.0a

First release of the document, derived from the earlier v4.2*x* document.

Version 5.0x-1.1a

Updated to include results of v5 specific accuracy calculations (prior version carried forward numbers from v4 analyses). Added averaging kernel information and ClO bias correction information as attachments to the document itself. Various minor modifications to text.

Contents

Chapter 1
Essential reading for users of MLS version 5.0 data

1.1 Scope and background for this document

This document describes the quality of the geophysical data products produced by version 5.0 of the data processing algorithms for the Earth Observing System (EOS) Microwave Limb Sounder (MLS) instrument on the Aura spacecraft. The intended audience is those wishing to make use of Aura MLS data for scientific study. This chapter, as its name implies, is considered essential reading for all users of MLS data.

Chapter 2 provides additional optional background information, outlining the algorithms used to generate the "Level 2" data (geophysical products reported along the instrument track) from the input "Level 1" data (calibrated microwave radiance observations). The bulk of the document, in Chapter 3, provides information on each of the MLS standard "Level 2" products. This includes quantification of resolution, precision, and accuracy, along with a description of data screening and usage rules and other caveats, notes on any anomalies, and some limited comparisons to other datasets. Key aspects of each product are summarized in Table 1.1.1. Finally, Chapter 4 (added in version 4.x-4.0 of this document) describes "Level 3" data products, derived from the Level 2 data, that provide easier access to collections of MLS observations (e.g., daily zonal means, monthly polar vortex averages) to facilitate additional studies using MLS observations. Users of these Level 3 data should still read the Chapter 1 material and the product-specific information in Chapter 3.

The v5.0*x* MLS data are the fifth "public release" of MLS data, having been preceded by versions 1.5, 2.2, 3.3/3.4, and 4.2. The v2.2 data are described in a series of validation papers published in a special issue of the *Journal of Geophysical Research* in 2007/2008. This document updates some findings from these papers for v5.0*x*, compares a limited subset of available v5.0*x* results to some of the previous data versions, and gives more general information on the use of MLS data. As always, those wishing to use MLS data are advised to consult the MLS science team concerning their intended use.

More information on the MLS instrument can be found in the document *An Overview of the EOS MLS Experiment* [*Waters et al.*, 2004]. A more general discussion of the microwave limb sounding technique and an earlier MLS instrument is given in *Waters et al.* [1999]. The theoretical basis for the Level 2 software is described in *Livesey and Snyder* [2004]. A crucial component of the Level 2 algorithms is the "Forward Model", which is described in detail in *Read et al.* [2004] and *Schwartz et al.* [2004]. The document *EOS MLS Retrieved Geophysical Parameter Precision Estimates* [*Filipiak et al.*, 2004] provides pre-launch estimates EOS MLS data precision. The impact of clouds on MLS measurements and the use of MLS data to infer cloud properties is described in *Wu and Jiang* [2004]. All the above documents and papers are available from the MLS web site (`https://mls.jpl.nasa.gov/`).

A subset of the information in those documents is also reported in a series of articles in the 2006 Aura special issue of the *IEEE Transactions on Geoscience and Remote Sensing*. Specifically, an overview of MLS is given in *Waters et al.* [2006], the algorithms that produce the data described here are reviewed in *Livesey et al.* [2006], *Read et al.* [2006], *Schwartz et al.* [2006], and *Wu et al.* [2006]. Other papers describe the calibration and performance of the various aspects of the MLS instrument [*Jarnot et al.*, 2006; *Pickett*, 2006; *Cofield and Stek*, 2006] and the MLS ground data system [*Cuddy et al.*, 2006]. The detailed validation of the MLS v2.2 dataset is described in a collection of papers in the "Aura Validation" special issue of JGR-Atmospheres (papers published in 2007 and 2008). These are cited in Chapter 3 on a product-by-product basis, along with some more recent references, in some cases.

Table 1.1.1: Summary of key information for each MLS standard product. Essential additional information is given in each product section of chapter 3.

Product	Useful vertical range / hPa	Quality threshold [1]	Convergence threshold [2]	Notes	Contact name
BrO	10–3.2	1.3	1.05	A,D,N	Luis Millán
CH3Cl	147–4.6	1.3	1.05	N	Michelle Santee
CH3CN	46–1.0	1.4	1.05	E,N	Michelle Santee
CH3OH	Not to be used pending further validation				Michelle Santee
ClO	147–1.0	1.3	1.05	B,D	Michelle Santee
CO	100–0.001 215–146	1.5	1.03	C	Hugh Pumphrey Michael Schwartz
GPH	83–0.00046 261–100	0.2 0.9	1.03	– C	Michael Schwartz
H2O	83–0.001 316–100	0.7	2.0	O,T C,O,T	Alyn Lambert William Read
HCl	100–0.32	1.2	1.05	R,T	Lucien Froidevaux
HCN	21–0.1	0.2	2.0	A,E,N,T	Hugh Pumphrey
HNO3	215–1.5	See text	See text	C	Michelle Santee
HO2	22–0.046	N/A	1.1	A,D,N	Luis Millán
HOCl	10–2.2	1.2	1.05	N	Lucien Froidevaux
IWC	215–83	See text	See text	B	Alyn Lambert
IWP	N/A	See text	See text	B	Alyn Lambert
N2O	100–0.46	0.8	2.0	R,T	Alyn Lambert
O3 [3]	100–0.001 261–121	1.0	1.03	C	Lucien Froidevaux Michael Schwartz
OH	32–0.0032	N/A	1.1	D	Luis Millán
RHI [4]	316–0.001	See text	See text	C,O,T	William Read
SO2	215–10	0.95	1.03	E	William Read
Temperature [5]	83–0.00046 261–100	0.2 0.9	1.03	– C	Michael Schwartz

Notes:

A Users should consider using alternative versions of this product, produced using different algorithms. See text.

B This product has significant biases in certain regions that may need to be accounted or corrected for in scientific studies. See text for details.

C Interference from clouds can affect this product at certain altitudes. See text for details.

D Biases in this product can be ameliorated (in selected conditions) by taking day/night differences. See text.

E At some altitudes, this product contains biases of a magnitude that render the product useful only for the study of “enhancement events” (e.g., volcanic plumes, extreme fire pollution). See text for details.

N This is a “noisy” product requiring significant averaging (e.g., monthly zonal mean). See text for details.

O This product contains significant outliers (e.g., spikes or oscillations) in some regions (typically from upper tropospheric clouds). These should be screened out as detailed in the text.

R The spectral region(s) used to retrieve this product has been revised at some point in response to a change in instrument behavior. Earlier versions of the MLS record used the original region.

T Care should be taken when considering long-term trends in measurements of this quantity. See text.

[1] Only use profiles with `Quality` *greater* than this value.

[2] Only use profiles with `Convergence` *less* than this value.

[3] File also contains a swath giving the column abundance above the (MLS-defined) tropopause.

[4] Relative humidity with respect to ice computed from the MLS H_2O and Temperature data.

[5] File also contains a swath giving tropopause pressure (WMO definition) inferred from MLS temperatures.

1.2 Overview of v5.0*x* and this document

The remainder of this chapter reviews issues that are considered *essential reading* for users of the v5.0*x* dataset. Chapter 2 details relevant aspects of the MLS instrument design and operations and the theoretical basis for the v5.0*x* Level 2 algorithms that are considered *background reading*.

Chapter 3 describes the data quality for "Standard" products from the MLS instrument for v5.0*x*. These are observations of vertical profiles of the abundance of BrO, CH_3Cl, CH_3CN, CH_3OH, ClO, CO, H_2O, HCl, HCN, HNO_3, HO_2, HOCl, N_2O, O_3, and OH and SO_2, along with temperature, geopotential height, relative humidity (deduced from the H_2O and temperature data), cloud ice water content and cloud ice water path, all described as functions of pressure. These profiles are mostly output on a grid that has a vertical spacing of six surfaces per decade change in pressure (~2.5 km), thinning out to three surfaces per decade above 0.1 hPa. Exceptions to this are water vapor, temperature, ozone and relative humidity which are on a finer 12 per decade grid from 1000 hPa to 1 hPa. Cloud ice water content is also reported on this fine grid, though these profiles do not extend to the stratosphere and mesosphere. The OH product maintains a 6 per decade grid spacing into the upper mesosphere. Horizontally the profiles are spaced by 1.5° great-circle angle along the orbit, which corresponds to about 160 km along track. The true vertical and along-track horizontal resolution of the products is typically somewhat coarser than the reporting grid described here. For some of the products, the signal to noise ratio is too low to yield scientifically useful data from a single MLS profile observation. In these cases, some form of averaging (e.g., weekly maps, monthly zonal means etc.) will be required to obtain more useful results.

In addition to these standard products, the algorithms also produce data for many "diagnostic" products. The bulk of these are similar to the standard products, in that they represent vertical profiles of retrieved species abundances. However, the information on these diagnostic products has typically been obtained from a different spectral region than that used for the standard products. These diagnostic products are not discussed in this document. Further information on these is available from the MLS science team.

At the time of writing, the current version of the data processing software is version 5.01, producing files labeled `v05-01`. The earlier v5.00 software, used to process some 1100 days-worth of MLS data is essentially similar, with two minor bugs, one causing processing software to fail on a handful of days, another related to the reporting of the "fill-value" (i.e., missing data flag) used for GPH, see section 3.8.

Any minor updates for bug fixes, or to reflect changes in input data such as the analysis fields used as *a priori* information for temperature will be referred to as v5.02, v5.03, etc. This version of the document is intended to be applicable to any v5.0*x* data files. More substantial changes at a later date (e.g., due to a change in the MLS instrument performance) may necessitate a larger change in the data processing software and/or its configuration. These will be numbered v5.1*x* etc., and will be accompanied by an updated version of this document (though not necessarily immediately, depending on the circumstances dictating the update).

1.3 MLS data validation status

As discussed above, a complete set of MLS validation papers describes the validation state of the earlier v2.2 data. The majority of the v2.2 MLS data products have, accordingly, completed "Stage 3 Validation" defined[1] as:

> *Product accuracy has been assessed. Uncertainties in the product and its associated structure are well quantified from comparison with reference in situ or other suitable reference data. Uncertainties are characterized in a statistically robust way over multiple locations and time periods representing global conditions. Spatial and temporal consistency of the product and*

[1] See `https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels/`

> *with similar products has been evaluated over globally representative locations and periods. Results are published in the peer-reviewed literature.*

Work, including that described in this document, has re-validated the v5.0*x* data, with the level of scrutiny for some (notably ozone and water vapor) establishing them as "Stage 4" validated, defined as:

> *Validation results for stage 3 are systematically updated when new product versions are released and as the time-series expands.*

1.4 Differences between MLS v5.0*x* data and earlier v4.x data

The MLS v5.0*x* data processing software includes a wide range of updates and changes, leading to differences ranging from significant to minor. Some of the most important are detailed below.

Partial amelioration of drifts in 190-GHz products (H_2O, N_2O, HCN): As discussed in *Hurst et al.* [2016] and *Livesey et al.* [2021], there are indications that the MLS H_2O product has been slowly drifting since ∼2010, at a rate of between 0.2–1%/year, depending on what record it is compared to (mainly frostpoint sonde or ACE-FTS) and the altitude range of interest. The MLS team has identified a slow change in one aspect of instrument calibration that accounts for some of this drift. Version 5.0 corrects for this calibration drift; the extent to which that correction fully accounts for the observed drift in Level 2 products remains to be studied as the v5.0*x* processing continues. The calibration trend also affects other species measured by the MLS 190-GHz subsystem, notably N_2O.

Correction of dry bias in upper tropospheric H_2O: As part of the work to identify and characterize the drift discussed above, the MLS team has also identified and largely corrected the source of a ∼20% dry bias below the tropopause.

Extension of N_2O product to 100 hPa: The v5.0*x* algorithms include a new retrieval for N_2O that reduces an issue seen at 100 hPa in earlier versions, rendering this pressure level suitable for scientific use. Note that the drift discussed above also affects N_2O, and unrealistic negative trends in this product in the lower stratosphere seem to have been reduced in the limited amount of data available for inspection to date.

Increased vertical range for some species: A new forward model has improved the performance of the O_3, H_2O, and CO retrievals in the upper mesosphere. Preliminary study has determined that the resulting improvements are sufficient to increase the vertical range over which these products are recommended for scientific use. However, further investigation is planned, and users are advised to employ caution in scientific studies considering those products in this altitude region.

In addition to these specific changes, changes in all products, including those not listed above, have resulted from updates to instrument calibration knowledge, and in indirect response to the larger changes detailed above. Note that the threshold values of "`Quality`" and "`Convergence`" (see below) to be used in data screening have been updated for some products. Also, the climatological fields used as *a priori* information in the retrievals of O_3, H_2O, HCl, HNO_3, and N_2O have been updated.

1.5 Aura MLS file formats, contents, and quality information

All the MLS Level 2 data files described here are available from the NASA Goddard Space Flight Center Earth Science Data and Information Services Center (GES-DISC, see `https://disc.gsfc.nasa.gov/`). The standard and diagnostic products are stored in the EOS MLS *Level 2 Geophysical Product* (L2GP)

Table 1.5.1: Additional swaths in specific standard product files.

Product	Additional swaths	Notes
HNO3	HNO3-190, HNO3-240	Nitric acid from the 190 and 240 GHz radiometers
IWC	IWP	partial Ice Water Path. (This file has no *a priori* swath)
O3	O3 column	Ozone column above the tropopause (see below)
RHI	UTRHI, UTRHI-APriori	"Single layer" relative humidity (see Section 3.20)
Temperature	WMOTPPressure	Tropopause (WMO definition, based on MLS temperature)

files. These are standard HDF-EOS (version 5) files containing swaths in the Aura-wide standard format. For more information on this format see *Craig et al.* [2003]. A sample reading function for the Interactive Data Language (IDL, version 6.1 or later required), known as `readl2gp.pro` may have been supplied with the data and is available from `https://mls.jpl.nasa.gov/data/readers.php` A reader for MATLAB (`readL2GP.m`) is also available at the same site.

The standard products are stored in files named according to the convention

```
MLS-Aura_L2GP-<product>_v05-00-c01_<yyyy>d<ddd>.he5
```

where `<product>` is `BrO`, `O3`, `Temperature`, etc. The files are produced on a one-day granularity (midnight to midnight, universal time), and named according to the observation date where `<yyyy>` is the four digit calendar year and `<ddd>` is the day number in that year (`001` = 1 January).

These files contain the corresponding standard product in an HDF-EOS swath given the same name as the product, e.g., "`H2O`". With the exception of IWC, each file also contains the *a priori* values for that product inside a second swath whose name ends with the substring "`-APriori`". HNO_3, IWC, O3, RHI, and Temperature files are special in that they carry extra standard or non-standard products, as detailed in Table 1.5.1.

The files contain an HDF-EOS swath given the same name as the product. In addition, the standard O_3 product files also contain swaths describing column abundances, and the standard Temperature file contains additional swaths describing tropopause pressure. As some L2GP files contain multiple swaths, it is important to ensure that the correct swath in the `L2GP` files is requested from the file. In the case where the "default" swath is requested (i.e., no swath name is supplied) most HDF software will access the one whose name falls earliest in ASCII order. This generally results in the desired result for all products. For example, for temperature, the standard "`Temperature`" product will be read in preference to the "`WMOTPPressure`" swath that gives tropopause pressures.

Each swath contains data fields `L2gpValue` and `L2gpPrecision`, which describe the value and precision (reported at 1σ) of the data, respectively. Data points for which `L2gpPrecision` is set negative or zero *should not be used*, as this flags that the resulting precision is worse than 50% of the *a priori* precision, indicating that instrument and/or the algorithms have failed to provide enough useful information for that point. In addition to these fields, fields such as `latitude` etc. describe geolocation information. The field `time` describes time, in the EOS standard manner, as the number of seconds (including leap seconds) elapsed since midnight universal time on 1 January 1993.

The `L2GP-DGG` ("Diagnostic products on a Geophysical Grid") file contains a large number of additional swath quantities. The vast majority of these are MLS diagnostic products that will be of little interest to most data users. A few that may be of interest to some users are detailed below.

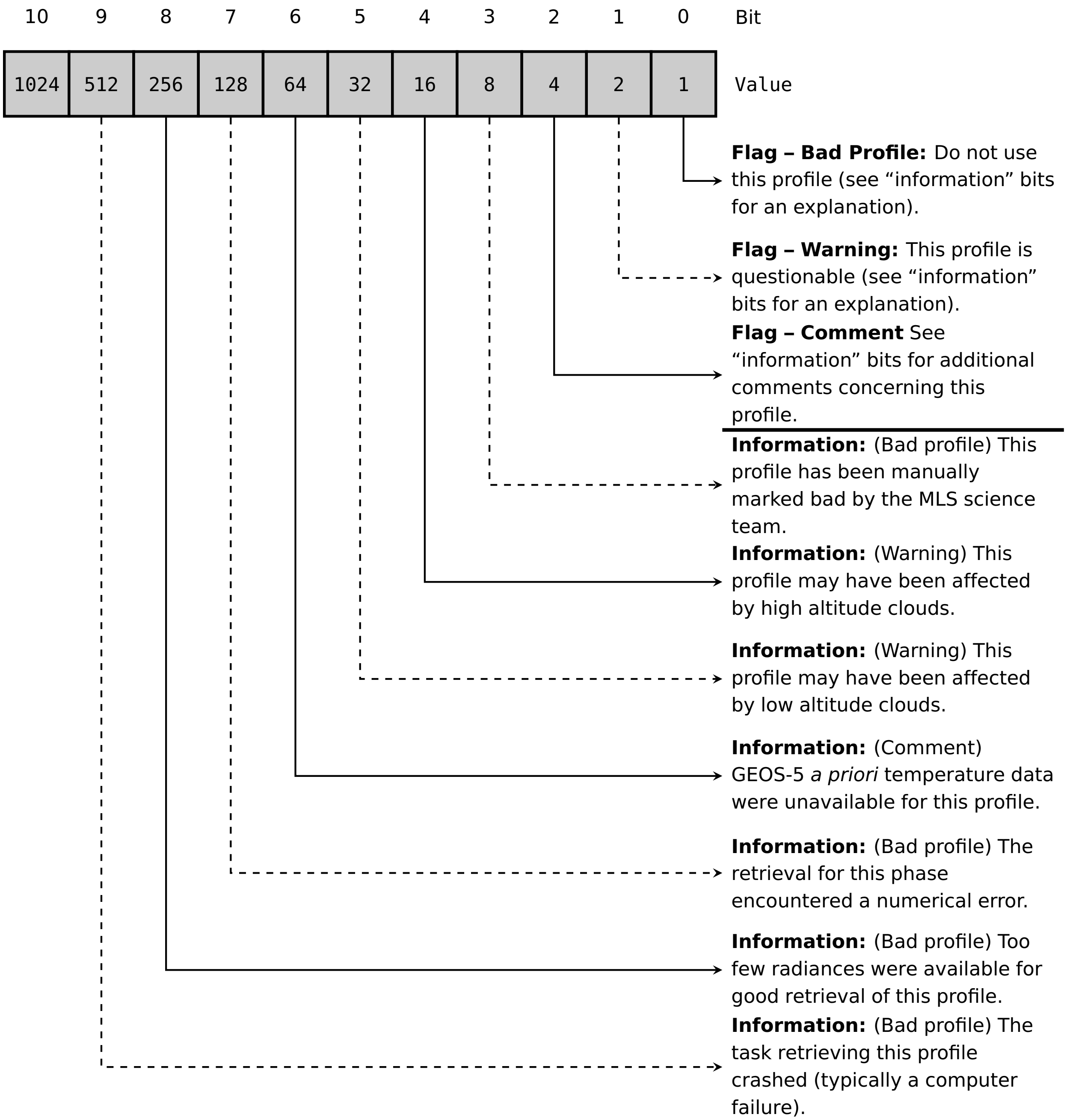

Figure 1.6.1: The meaning of the various bits in the `Status` field.

1.6 Additional information given in the `Quality`, `Convergence` and `Status` fields

In addition to the data and their estimated precisions, three quality metrics are output for every profile of each product. The first, called `Quality`, gives a measure of the quality of the product based on the fit achieved by the Level 2 algorithms to the relevant radiances. Larger values of `Quality` generally indicate better radiance fits and therefore more trustworthy data. Values of `Quality` closer to zero indicate poorer radiance fits and therefore less trustworthy data. The value of `Quality` to be used as a

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"threshold" for rejecting data in scientific studies varies from product to product, and is given later in this document.

The second quality metric is called `Status`. This is a 32 bit integer that acts as a bit field containing several "flags". Figure 1.6.1 describes the interpretation of these flags in more detail. The first three bits (bits 0, 1, and 2) are "flagging" bits. If the first bit ("bad profile") is set it indicates that the profile *should not be used in any scientific study*. Accordingly, any profile for which `Status` is an odd number should not be used. The second bit ("warning") indicates that data are considered questionable for some reason, while the third ("comment") indicates the data are noteworthy in some manner that does not rise to the level of a "warning". Higher bits give more information on the reasons behind the setting of the first three bits. So, for example, a value of `Status` of 18 (2+16) indicates that the data are questionable ($2 \equiv$ bit 2) because of the possible presence of high altitude clouds ($16 \equiv$ bit 4).

The most commonly set information bits are the "high altitude cloud" and "low altitude cloud" bits. These indicate that the data have been marked as questionable because the Level 2 software judged that the measurements may have been affected by the presence of clouds (clouds alone will never cause a profile to be marked as not to be used, i.e., with odd `Status`). The implications of this vary from product to product and, more importantly, height to height. For example, situations of either "low cloud" or "high cloud" typically have very little impact on the quality of stratospheric data. Further details of the implications of these flags are given later in this document on a product by product basis.

The third diagnostic field `Convergence` describes how the fit to the radiances achieved by the retrieval algorithms compared to the degree of fit to be expected. This is quantified as a ratio of an aggregate χ^2 value to that predicted based on the assumption of a linear system [*Livesey et al.*, 2006]. Values around unity indicate good convergence and the threshold values above which profiles should not be used are given on a product by product basis later in this document.

1.7 An important note on negative values

Some of the MLS observations are "noisy" in nature. A consequence of this is that negative values may often be reported for species mixing ratios. It is important that such values *not be ignored or masked*. Ignoring such values will automatically introduce a positive bias into any averages made of the data as part of scientific analysis. Water vapor is retrieved using a logarithmic basis (both vertically and horizontally, as discussed in Section 1.9). Accordingly, no negative water vapor abundances are produced by v5.0*x*.

1.8 Averaging kernels for MLS v5.0*x* profiles

As is common for remote sounding instruments, consideration of the "Averaging Kernel" [e.g., *Rodgers*, 2000] can be useful in some scientific studies. However, the relatively high vertical resolution of the MLS observations (compared, for example, to those from nadir sounding composition instruments) allows for many scientifically useful studies to be undertaken without reference to the averaging kernels. This section reviews the role averaging kernels play in comparing MLS measurements to other observations and/or model fields and describes how to obtain representative kernels for the v5.0*x* data.

The averaging kernel matrix $\mathbf{A}$ relates the retrieved MLS profiles (given by the vector $\hat{\mathbf{x}}$) to the "true" atmospheric state (the vector $\mathbf{x}$) according to

$$\mathbf{A} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}}. \tag{1.1}$$

Rows of the $\mathbf{A}$ matrix accordingly describe the contributions of the true atmospheric profile to the given level in the retrieved profile. The figures later in this document show these rows as individual colored lines.

Given an independent observation or model estimate of an atmospheric profile $\mathbf{x}$, the averaging kernels, in combination with the MLS *a priori* profile $\mathbf{x}_a$, can be used to linearly approximate the profiles that MLS would observe, were the true profile to be in the state given by $\mathbf{x}$, according to

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}[\mathbf{x} - \mathbf{x}_a] \tag{1.2}$$

It is assumed here that the true profile uses the same vertical grid as the MLS data product in question (Section 1.9 discusses this issue further). Note that this linearization is about the *a priori* state, so the blurring by the averaging kernels is only of the difference between truth and *a priori*. As of MLS version v04.2*x*, the *a priori* profile for each MLS observation is available within each of the standard product files, in swaths named according to the product, with the suffix "`-APriori`" (note the hyphen). Examples are "`Temperature-APriori`" and "`O3-APriori`". This information can also be obtained from the MLS `L2GP-DGG` files. In the case of water vapor, where a logarithmic interpolation is used for the profile, the calculations in Equation 1.3 should be performed in log space, i.e., with $\mathbf{x}$ and $\mathbf{x}_a$ containing logarithm of the given H_2O mixing ratio (leaving the $\mathbf{A}$ matrix as supplied).

The MLS retrieval algorithms are "tomographic" in nature, in that they use information from multiple consecutive limb scans to simultaneously estimate the 2-dimensional (along-track and vertical) state of the atmosphere over multiple Level 2 profiles (see Section 2.2). Formally therefore, the MLS averaging kernels describe the smoothing in both the horizontal and vertical directions. Archived two dimensional (2-D) averaging kernels capture this dependence, containing the partial derivatives of each level of a given profile to the truth at all levels of a block of eleven profiles centered on the location of the retrieved profile. These full kernels can be "collapsed" in the horizontal, to provide a single vertical averaging kernel for each product (similar to those provided for many nadir sounding instruments), corresponding to the single-profile view of the retrieval described in the preceding paragraph. Similarly, contributions from adjacent profiles to the retrieved values at each level may be collapsed in the vertical, to provide horizontal averaging kernels that capture the horizontal resolution of the product. Vertical and horizontal kernels are shown for each product in Chapter 3.

The MLS averaging kernels typically change little with latitude, season, or atmospheric state. Accordingly, two representative kernels are shown for each product, one for the tropics and one for polar winter conditions. These representative kernels are available to users, as described below. If variability in the averaging kernels is a concern, comparison of $\hat{\mathbf{x}}$ profiles obtained using each of the two kernels (typically representing extreme cases) can provide a quantitative estimate of the magnitude of differences introduced by kernel variations.

Representative vertical, horizontal and 2-D averaging kernels have been archived for each MLS standard product on the MLS website, and are also attached to this document (see Appendix A). Two sets of kernels are provided, each comprising five files corresponding to five broad latitude bands. One set contains 1-D (horizontal and vertical) kernels, the other the full 2-D kernels, making ten files in all. Each file contains kernels (either 1-D or 2-D) for each of the MLS standard products for the given latitude band. Again, as the averaging kernels vary little with latitude, a file for a single latitude will generally be globally representative. These kernels were calculated from simulated MLS data for a single day (based on output from the SLIMCAT model for February 20, 1996). The resolution of most MLS products varies little seasonally, as can be inferred from the minimal hemispheric variability within the single day used to compute the kernels. These files can be read as either NetCDF or HDF-5 files, for which interfaces exist in many high-level analysis environments such as IDL, Python and Matlab. These files contain multi-dimensional arrays, with dimensions named `RetrievalLevel`, `TruthLevel` and `TruthPhi`. The latter is the along-track horizontal coordinate used in the MLS retrievals, within which profiles are spaced 1.5° great circle distance apart.

In most cases, consideration of the 1-D vertical averaging kernels is likely sufficient to quantify the impact of the finite MLS resolution on a scientific study. In a column-major language (e.g., Matlab, IDL,

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Table
BrO S T
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CH_3CN S T
CH_3OH S T
ClO S T
CO S T
GPH S T
H_2O S T
HCl S T
HCN S T
HNO_3 S T
HO_2 S T
HOCl S T
IWC S T
IWP S T
N_2O S T
O_3 S T
OH S T
RHI S T
SO_2 S T
T S T
Lvl 3

Fortran), the 1-D vertical **A** matrix will be dimensioned [`RetrievalLevel`, `TruthLevel`], and the truth profiles should be multiplied by averaging kernels from the left (as in Equation 1.3, above). In a row-major language (e.g., C, Numpy), the order of dimensions in **A** is reversed, and the averaging kernels should be multiplied by truth from the right. Horizontal averaging kernels (`avkh`), have size $N_{\text{lev}} \times 11$ in a column major and $11 \times N_{\text{lev}}$ in a row major environment, where N_{lev} is 55 for a high-resolution MLS product (Temperature, GPH, water vapor, and ozone), and 37 for most other products. The side on which `avkh` has the 11-element dimension is the side against which truth profiles should be multiplied for all horizontal averaging kernels.

The 2-D averaging kernels give weights for every level of every nearby (within ±5) profile of truth, so in a row-major language are $11 \times N_{\text{lev}} \times N_{\text{lev}}$ and in column-major language will be $N_{\text{lev}} \times N_{\text{lev}} \times 11$. To perform the convolution, blocks of eleven adjacent truth and *a priori* profiles centered on the retrieved profile location are unwrapped into length $N_{\text{lev}} \times 11$ vectors, $\mathbf{X}$ and $\mathbf{X}_a$. The 2-D averaging kernel, $\mathbf{A}_{\text{2D}}$, is reshaped into a two dimensional matrix $N_{\text{lev}} \times (N_{\text{lev}} \times 11)$ and the retrieved state is estimated as

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{A}_{\text{2D}} \left[\mathbf{X} - \mathbf{X}_a \right]. \tag{1.3}$$

Vertical averaging kernels for each product for 70°N and the equator are also available as text files, in the format used for previous MLS releases. These files are named according to

```
MLS-Aura_L2AK-<product>-<case>_v05-00_0000d000.txt
```

where `<case>` is `Eq` or `70N` for the equator and 70°N, respectively (or `Day` and `Night` for OH, see Section 3.19). These files, for all products, are available as a single tar archive from the MLS web site at `https://mls.jpl.nasa.gov/eos-aura-mls/data-products/averaging-kernels/`.

These files contain comment lines (prefixed with a semicolon) describing their format. The first non-comment line gives the name of the product and the number of levels in the vertical profile. A list of the pressure levels in the profile (matching those in the L2GP files) is then given, followed by all the values of the averaging kernel matrix, with the row index (the level in the retrieved profile) varying most rapidly.

As discussed above, the MLS profile pressures are typically not those of the observation or model dataset to which the comparison is being made. In many cases, particularly where the resolution of the other dataset is comparable to that of the MLS profiles, a simple interpolation is the most practical manner in which to transform the other dataset into the **x** profile space. However, we note that more formal approaches have been described [*Rodgers and Connor*, 2003] for the case where the comparison dataset is also remotely sounded and has an averaging kernel. In cases where the comparison dataset has high vertical resolution (e.g., sonde or Lidar observations), an additional consideration is described in the following section.

1.9 Considerations for comparisons with high vertical resolution datasets

The MLS Level 2 data describe a piecewise linear representation of vertical profiles of mixing ratio (or temperature, GPH, etc.) as a function of pressure, with the tie points given in the `L2GP` files (in the case of water vapor, the representation is piecewise linear in log mixing ratio). This contrasts with some other instruments, and model output datasets, which report profiles in the form of discrete layer means. This interpretation has important implications that may need to be considered when comparing profiles from MLS to those from other instruments or models, particularly those with higher vertical resolution.

It is clearly not ideal to compare MLS retrieved profiles with finer resolution data by simply "sampling" the finer profile at the MLS retrieval surfaces. One might expect that instead one should do some

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

linear interpolation or layer averaging to convert the other dataset to the MLS grid. However, in the MLS case where the state vector describes a profile at infinite resolution obtained by linearly interpolating from the fixed surfaces, it can be shown that the appropriate thing to do is to compare to a least squares fit of the non-MLS profile to the lower resolution MLS retrieval grid.

Consider a high resolution profile described by the vector $\mathbf{z}_h$, and a lower resolution MLS retrieved profile described by the vector $\mathbf{x}_l$. We can construct a linear interpolation in log pressure that interpolates the low resolution information in $\mathbf{x}_l$ to the high resolution grid of $\mathbf{z}_h$. We describe that operation by the (typically highly sparse) $n_h \times n_l$ matrix $\mathbf{H}$ such that

$$\mathbf{x}_h = \mathbf{H}\mathbf{x}_l \tag{1.4}$$

where $\mathbf{x}_h$ is the high resolution interpolation of the low resolution $\mathbf{x}_l$. It can be shown that the best estimate profile that an idealized MLS instrument could obtain, were the true atmosphere in the state described by $\mathbf{z}_h$, is given by

$$\mathbf{z}_l = \mathbf{W}\mathbf{z}_h \tag{1.5}$$

where

$$\mathbf{W} = \left[\mathbf{H}^{\mathrm{T}}\mathbf{H}\right]^{-1}\mathbf{H}^{\mathrm{T}} \tag{1.6}$$

In other words, $\mathbf{z}_l$ represents a least squares linear fit to $\mathbf{z}_h$. This operation is illustrated by an example in Figure 1.9.1. Precision uncertainty on high resolution measurements may be similarly converted to the MLS grid by applying

$$\mathbf{S}_l = \mathbf{W}\mathbf{S}_h\mathbf{W}^{\mathrm{T}} \tag{1.7}$$

where $\mathbf{S}_h$ is the covariance of the original high resolution data (typically diagonal) and $\mathbf{S}_l$ is its low resolution representation on the MLS pressure grid. Following this transfer of the high-resolution profile onto the state vector vertical grid, the profile can be multiplied by the averaging kernels, as described above, according to equation 1.3.

In some cases, the application of this least-squares “smoothing” is as important, if not more important, than the application of the averaging kernels described above. This is particularly true when the averaging kernels are close to delta functions, indicating that the vertical resolution is comparable to the retrieved profile level spacing.

In the case of water vapor, where a logarithmic vertical basis is used, the $\mathbf{x}$ and $\mathbf{z}$ vectors should describe the logarithm of the mixing ratio.

1.10 A note on the HCl measurements in v5.0*x*

Starting in February 2006, the primary MLS band for measuring HCl (specifically the HCl^{35} isotopologue) (`R4:640.B13F:HCl` or “band 13”) began to exhibit symptoms of aging and was deactivated to conserve life. This is likely to be due to a radiation susceptibility issue for a batch of transistors identified shortly before launch. Useful observations of HCl are still made with the adjacent band (`R4:640.B14F:O3` or “band 14”) which, as can be seen from Figures 2.1.1 and 2.1.2 also observe the HCl^{35} line (and a smaller line for the HCl^{37} isotopologue); these retrievals produce the v5.0*x* standard HCl product (as they did for v4.2*x* HCl).

In order to avoid undesirable discontinuities in the v5.0*x* HCl dataset, the band 13 radiances are not considered in the retrieval of the standard HCl product, even on days for which it was active. For days prior to the 16 February 2006 deactivation of band 13, and the few subsequent days when band 13 has been (or may be) reactivated, the v5.0*x* algorithms also produce a second HCl product (in the `HCl-640-B13` swath in the `L2GP-DGG`) file which includes the band 13 radiances, giving a product with improved precision and resolution in the upper stratosphere and mesosphere. See Section 3.10 for more information.

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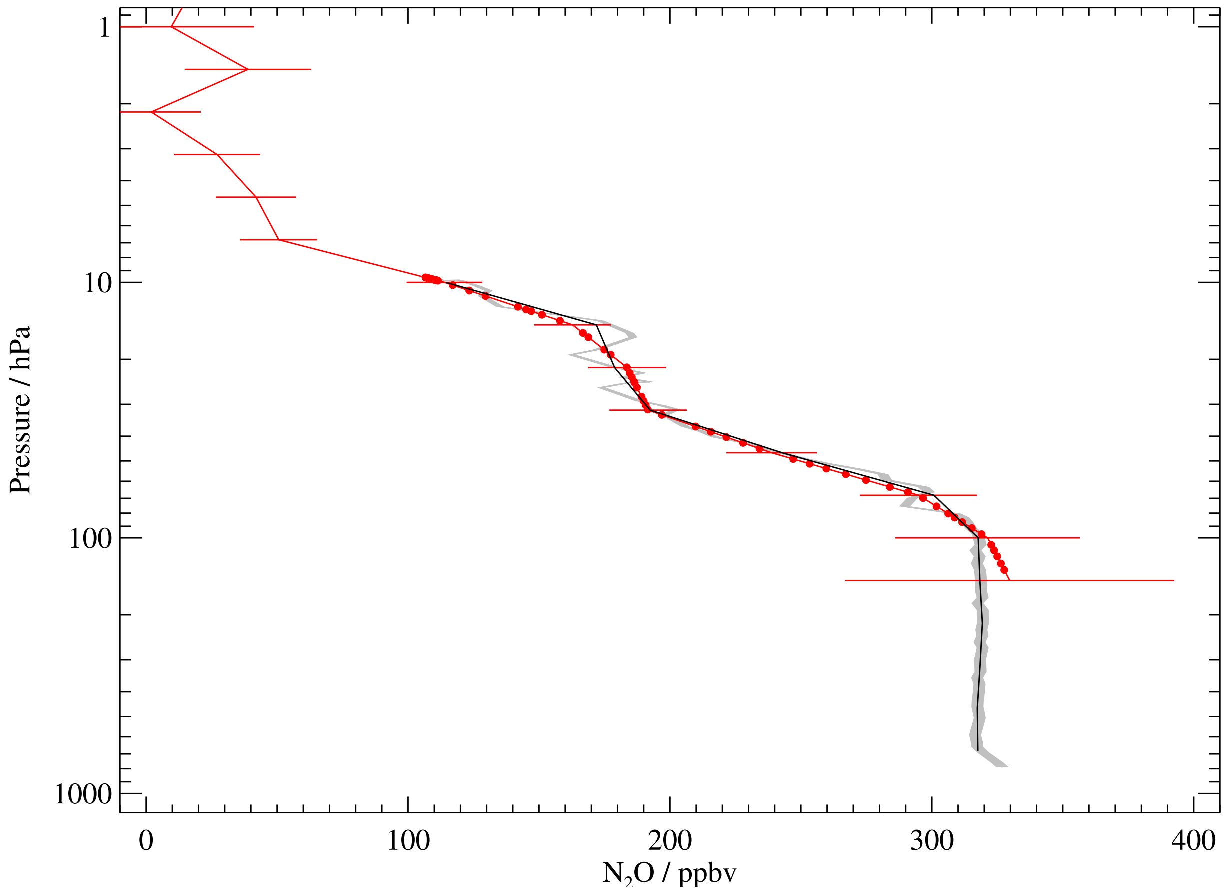

Figure 1.9.1: Comparisons of MLS (v1.5) N_2O observations with in-situ balloon data (courtesy of J. Elkins). The raw balloon data ($\mathbf{z}_h$) are shown as the grey shaded region (shading indicates precision). A coincident MLS profile ($\mathbf{x}_l$) is shown in red with the red error bars indicating precision. The red dots show the MLS data linearly interpolated to the balloon pressures using the $\mathbf{H}$ matrix (i.e., $\mathbf{x}_h$ from equation 1.4). The black line shows the "least squares" interpolation of the balloon data onto the MLS grid using the $\mathbf{W}$ matrix as described in the text (i.e., $\mathbf{z}_l$ from equation 1.5). The black line therefore represents the closest possible match at this resolution to the original grey line, and is the appropriate quantity to compare to the red MLS profile, and to be multiplied by the averaging kernels for formal comparison.

As discussed in Section 3.10, while the band 14 and band 13 data show very good agreement in the lower stratosphere, they disagree on the magnitude of the declining trend in upper stratospheric HCl (reflecting cuts in emissions of ozone depleting substances). At these high altitudes the HCl line is significantly narrower than the single channel in band 14 in which it resides, whereas the band 13 channels (by design, as this band was targeted to HCl) resolve the line shape. Accordingly, the band 13 trend is judged to be the more accurate one.

1.11 A note on N_2O measurements in v5.0*x*

The preferred MLS band for measuring N_2O (band 12 in the 640 GHz region, `N2O-640`) began to show signs of aging in June 2013 (although more slowly than the rapid decline observed in the HCl band 13 in 2006). Band 12 was subsequently turned off on August 6, 2013. However, the level-2 processing stream for the N_2O standard product in v3.x was switched to output the band 3 (190 GHz, `N2O-190`) retrieval on 7 June 2013 and later data for `N2O-640` are not recommended for scientific use.

For v5.0*x*, as similarly for v4.2*x*, the band 3 (190 GHz, `N2O-NitrousOxide`) retrievals are used as the standard product from launch, whereas the band 12 (640 GHz, `N2O-640`) retrieval is now only available in the `N2O-640` swath in the `L2GP-DGG` file.

1.12 A note on OH measurements in v5.0*x*

The MLS OH measurements derive from observations in the 2.5-THz region of the spectrum. The local oscillator signal driving the MLS 2.5-THz radiometers is provided by a methanol laser (pumped by a CO_2 laser). In December 2009, following more than five years of operation, this laser began to show signs of aging and was temporarily deactivated (prior to the 2004 Aura launch, the expected lifetime of this laser was only eighteen months).

Upper stratospheric and mesospheric OH is strongly affected by solar activity [*Wang et al.*, 2013], which was low during the solar 11-year minimum in 2009. In order to conserve the remaining lifetime of the THz instrument for valuable measurements when the Sun becomes more active, we suspended OH measurements from December 2009. The THz subsystem was reactivated for 30 day periods around August each year between 2011 and 2014, providing coverage of a full 11-year solar cycle. However, due to the aging of the instrument, OH data acquired in the 2014 period are significantly noisier than the previous years and have poor spatial coverage at mid-low latitudes. Any remaining life in the MLS THz subsystem is being conserved pending unusual solar activity.

Chapter 2
Background reading for users of MLS version 5.0 data

2.1 Aura MLS radiance observations

Figures 2.1.1 and 2.1.2 show the spectral coverage of the MLS instrument. The instrument consists of seven radiometers observing emission in the 118 GHz (R1A and R1B), 190 GHz (R2), 240 GHz (R3), 640 GHz (R4) and 2.5 THz (R5H and R5V) regions. With the exception of the two 118 GHz devices, these are "double sideband" radiometers. This means that the observations from both above and below the local oscillator frequencies are combined to form an "intermediate frequency" signal. In the case of the 118-GHz radiometers, the signals from the upper sideband (those frequencies above the $\sim$126 GHz local oscillator) are suppressed. These intermediate frequency signals are then split into separate "bands". The radiance levels within these bands are quantified by various spectrometers.

In operation, the instrument performs a continuous vertical scan of both the GHz (for R1A–R4) and THz (R5H, R5V) antennæ from the surface to about 90 km in a period of about 20 s. This is followed by about 5 s of antenna retrace and calibration activity. This $\sim$25 s cycle is known as a *Major Frame* (MAF). During the $\sim$20 s continuous scan, radiances are reported at 1/6 s intervals known as *Minor Frames* (MIFs).

2.2 Brief review of theoretical basis

The Level 2 algorithms implement a standard *Optimal Estimation* retrieval approach [*Rodgers*, 1976, 2000] that seeks the "best" value for the state vector (the profiles of temperature and abundances) based on an optimal combination of the fit to the MLS radiance observations, *a priori* estimates of the state vector (from climatological information and, for temperature in the troposphere and lower stratosphere, analysis fields), and constraints on the smoothness of the result. This fit must often be arrived at in an iterative manner because of the non-linear nature of the Aura MLS measurement system.

An innovative aspect of the retrieval algorithms for Aura MLS arises from taking advantage of the fact that the MLS instrument looks in the forward direction from the spacecraft. Figure 2.2.1 reviews the Aura MLS measurement geometry and shows that each radiance observation is influenced by the state of the atmosphere for several consecutive profiles. In the v5.0*x* Level 2 algorithms, the state vector consists of "chunks" of several profiles of atmospheric temperature and composition, which are then simultaneously retrieved from radiances measured in a similar number of MLS scans. Results from these "chunks" are then joined together to produce the products at a granularity of one day (the chunks overlap in order to avoid "edge effects").

The retrieval state vector consists of vertical profiles of temperature and composition on fixed pressure surfaces. Between these fixed surfaces, the forward models assume that species abundances and temperature vary from surface to surface in a piecewise-linear fashion (except for the abundance of H_2O, which is assumed to vary linearly in the logarithm of the mixing ratio). This has important implications for the interpretation of the data as was described in Section 1.9. In addition to these profiles, the pressure at the tangent point for the mid-point of each minor frame is retrieved, based on both radiance observations and knowledge of tangent point height from the MLS antenna position encoder and the Aura spacecraft ephemeris and attitude determination.

Most of the MLS data products are deduced from observations of spectral contrast, that is, variations in radiance as a function of frequency for a given limb pointing. Many of the systematic errors in the MLS measurement system manifest themselves as a spectrally flat or slowly spectrally varying error in

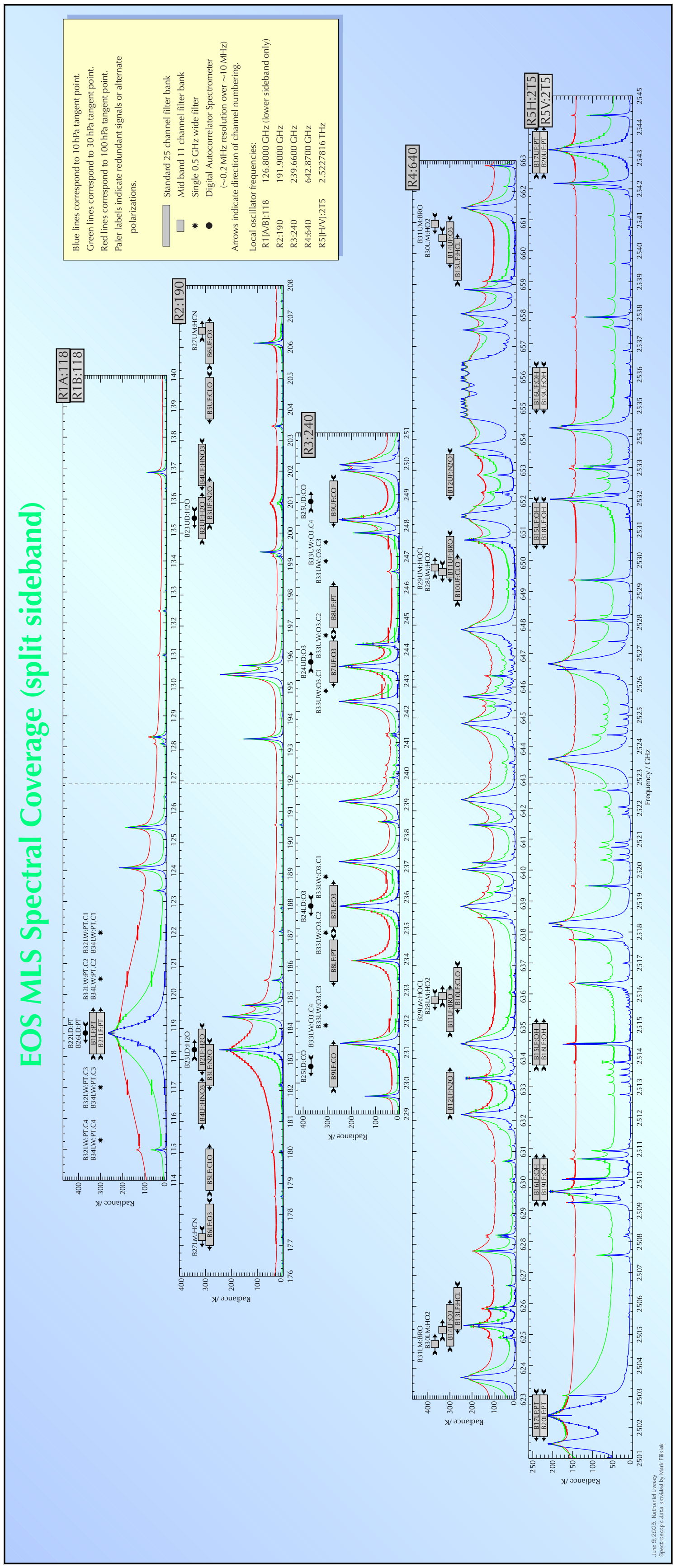

Figure 2.1.1: The five panels show the spectral regions covered by the MLS radiometers. The grey boxes and other symbols denote the position of the various "bands" observed within the spectral regions covered by each radiometer.

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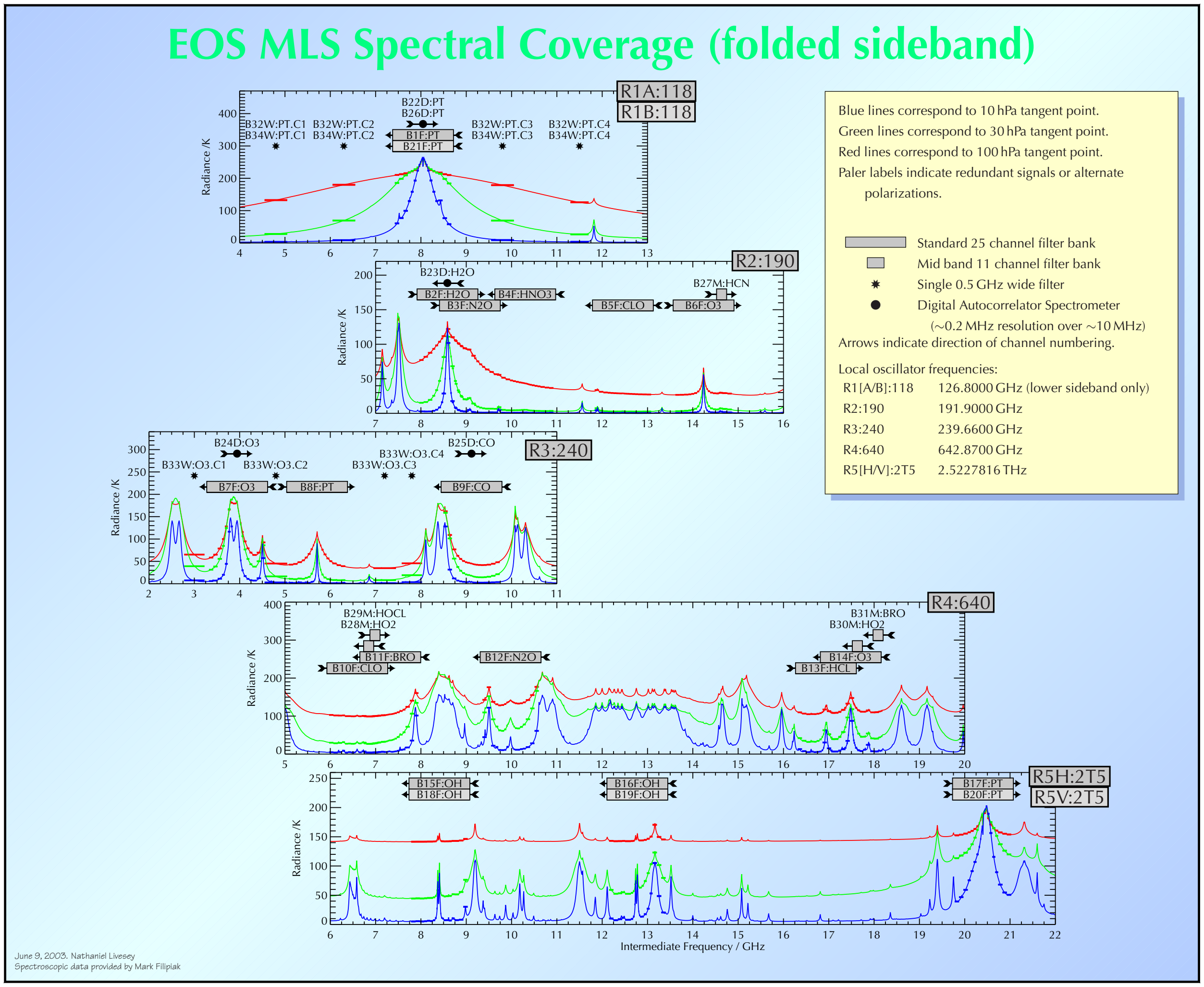

Figure 2.1.2: This is similar to figure 2.1.1, except that x-axes represent "intermediate frequency". The signal at each intermediate frequency represents a sum of the signals observed at that frequency both above and below the local oscillator (below only in the case of the 118 GHz receivers.)

radiance. This is true of effects arising both from the instrument (such as gain and offset during the limb scan) and from the "forward model" (such as knowledge of continuum emission and the impact of some approximations made in the forward model in order to increase its speed). In order to account for such effects, the v5.0*x* algorithms also retrieve spectrally flat (or slowly spectrally varying) corrections to the MLS radiances, either in terms of an additive radiance offset or an additive atmospheric extinction.

2.3 The Core, CorePlusR*n* approach

2.3.1 The need for separate "phases"

Many aspects of the MLS measurement system are linear in nature. In other words, there is a linear relationship between changes in aspects of the atmospheric state and consequent changes in the MLS radiance observations. However, there are some components of the state vector whose impact on the radiances is non-linear. The most non-linear of these is the estimate of the tangent pressure for each MIF of observation. The impact of water vapor in the upper troposphere on the MLS radiance observations is also highly non-linear. Solving for these aspects of the state vector therefore requires several iterations.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

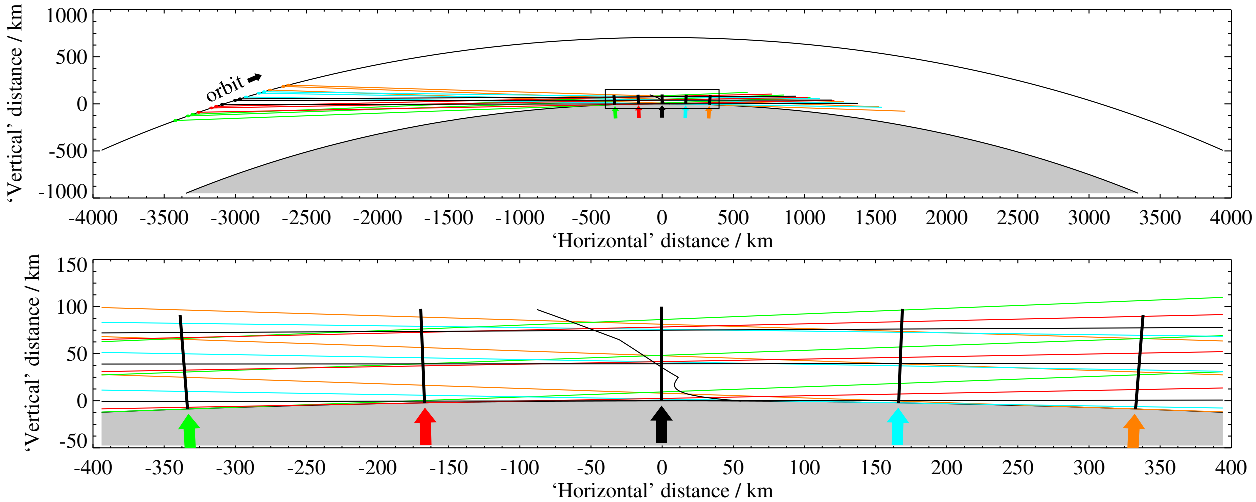

Figure 2.2.1: The top diagram shows a section of one orbit. Three of the 120 limb ray paths per scan are indicated by the "horizontal" lines. The lower diagram shows an expansion of the boxed region above. The straight radial lines denote the location of the retrieved atmospheric profiles. The limb ray scan closest to each profile is that whose color is the same as that of the arrow underneath. The thin black line under the central profile indicates the locus of the limb tangent point for this scan, including the effects of refraction.

The computational effort involved in retrieval and forward models scales very rapidly (arguably as high as cubically) as a function of the size of the measurement system (i.e., the number of elements in the state and measurement vectors). Thus it is desirable to simplify retrievals involving strongly non-linear variables to a small subset of the complete system, in order to cut down on the effort involved in retrievals that require many iterations.

For this and other reasons, most retrieval algorithms are split into *phases*. In the case of the MLS v5.0*x* retrievals, there are many such phases. The first group of phases (collectively known as "Core") use the 118 GHz and 240 GHz observations of O_2 and $O^{18}O$, respectively, to establish estimates for temperature and tangent pressure. Upper tropospheric 190 GHz radiances are used in these early phases to establish a first order estimate of upper tropospheric humidity. The "Core" phases also include "cloud screening" computations (based on differences between observed and estimated clear-sky radiances). These identify minor frames where radiances in a given radiometer have been subject to significant (and currently poorly modeled) cloud scattering. Such minor frames are ignored in v5.0*x* processing in certain radiometers. Including information in such cloud-contaminated conditions is a goal for future MLS data processing versions.

The "Core", phases are followed by phases such as `CorePlusR3` and `CorePlusR5`, where composition profiles are retrieved from a given radiometer. Sometimes (e.g., for `CorePlusR3`) these later phases continue to retrieve temperature and pressure, continuing using information from the 118 GHz radiometers, as in "Core". In other phases (e.g., the `CorePlusR2` and `CorePlusR4` families of phases), the 118 GHz information is neglected and temperature and pressure are constrained to the results of "Core". This choice is made based on extensive testing aimed at maximizing the information yield from MLS while minimizing the impact of inevitable systematic disagreements among the different radiometers, introduced by uncertain spectroscopy and/or calibration knowledge.

Table 2.3.1 describes the phases in more detail. Many products (e.g., ozone) are produced in more than one phase. All the separate measurements of these species are produced as diagnostic quantities, and labeled according to the spectral region from which they originated. For example, the ozone obtained from the `CorePlusR2` retrieval is known in the v5.0*x* dataset as `O3-190`. In v5.0*x* in order to

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

reduce confusion for users of MLS data, the algorithms also output "standard products", which is typically a copy of one of the products from the `CorePlusRn` phases. For example, the "standard" chlorine monoxide product is a copy of the `ClO-640` product. In the case of v5.0*x* nitric acid, the standard product represents a hybrid of the results from two phases. Details of which standard product is obtained from which phase are given in Table 2.3.2.

2.4 Forward models used in v5.0*x*

The retrieval algorithms in v5.0*x* make use of a variety of different forward models. The most accurate is the so-called "full" forward model described in *Read et al.* [2004] and *Schwartz et al.* [2004]. This is a hybrid line-by-line and channel averaged model that computes radiances on appropriate grids of frequency and tangent pressure that are then convolved with the MLS frequency and angular responses.

This model is generally rather time consuming, although for some comparatively "clean" spectral regions the computational burden is small enough that the full forward model can be used in the operational retrievals. Further, in the years since the Aura launch, computational capabilities have improved significantly, allowing for wider use of the full forward model in the MLS retrievals.

For some of the MLS channels, a simpler "Linearized" forward model can be used to estimate either radiances, or more typically the "Jacobian" (also know as "weighing function") information. The Linearized model invokes a simple first-order Taylor series to estimate radiances as a function of the deviation of the state from one of several pre-selected representative states. The inputs to this model are pre-computed radiances and derivatives corresponding to the pre-selected states, generated by "off-line" runs of the full forward model.

In addition, a "cloud" forward model can be invoked to model the effects of scattering from cloud particles in the troposphere and lower stratosphere [*Wu and Jiang*, 2004]. This model was used in the simulation of radiances based on known model atmospheres for the v5.0*x* testing, but is not invoked in the v5.0*x* retrieval algorithms (the handling of clouds is described in more detail in Section 2.5).

2.5 The handling of clouds in v5.0*x*

Thin clouds and atmospheric aerosols do not affect MLS atmospheric composition measurements as the typical particle sizes are much smaller than the wavelengths of the radiation being observed. The MLS v5.0*x* algorithms can reliably retrieve composition in moderately cloudy cases (having small limb radiance perturbations) and in the case of the Core+R3 retrieval this is handled by retrieving a frequency squared dependent extinction (including background atmospheric absorption from N_2, H_2O and unknown emitters). In the other retrieval phases, by contrast, a spectrally-flat baseline is used. Thick clouds can affect the MLS radiances beyond the modeling capability of this approach, mainly through scattering processes. Such situations and the affected radiances are excluded from the retrievals, or their influence down-weighted.

The first aspect of handling clouds in v5.0*x* is therefore the flagging of radiances that are believed to be significantly contaminated by cloud effects. To determine if a cloud is present in each MLS radiance measurement, we estimate the so-called cloud-induced radiance (T_{cir}). This is defined as the difference between the measured radiance and the radiance from a forward model calculation assuming clear-sky conditions. Specific window channels (those that are most transparent deepest into the atmosphere) in each radiometer are chosen to set these flags.

Cloud screening in the Core+R2 and Core+R3 phases is based on determining the highest altitude limb view contaminated by cloud signals and either rejecting all radiances below that altitude or, in the case of less impacted channels, inflating their estimated radiance precisions. Clouds are detected by a combination of a radiance fit χ^2 quantity from Band 8 (240 GHz isotopic oxygen line) retrieval of temperature and pointing, and a cloud induced radiance calculation, also using 240 GHz measurements.

Table 2.3.1: The phases that form the v5.0x retrieval algorithms.

Phase	Target species[1]	Measurements	Comment
InitPTan	T, pTan (GHz), GPH	R1A & R1B (118 GHz)	Initial estimate of P/T, lower limit 261 hPa
InitR2	H_2O, N_2O, CH_3CN, HCN, ClO, HNO_3, O_3, SO_2	R2 (190 GHz)	Initial trace gas estimator, lower limit 100 hPa
R3InitRHi	RHi, T_{cir}	R3 (240 GHz)	Retrieves RHi profile from 316 hPa and up, used mostly for "near field" cloud detection and to compute R3 T_{cir}
CloudDetector	none	R3 (240 GHz)	Determines cloud screening for R2 (190 GHz) and R3 (240 GHz)
FinalPTan	T, pTan (GHz), GPH	R1A & R1B (118 GHz), R3 (240 GHz)	Best P/T retrieval, lower limit 261 hPa
InitLowCloud	T_{cir}	All radiometers	Determines cloud flags for all phases
InitRHi	UT RHi	R2 (190 GHz)	Retrieve RHi in a ~6 km-layer centered 400–600 hPa. Uses only saturated radiances
InitUTH	Upper tropospheric H_2O	R2 (190 GHz)	Low vertical resolution (6/decade)
CorePlusR3	T, pTan (GHz), GPH, O_3[2], CO, HNO_3, SO_2, RHi[b]	R1A & R1B (118 GHz), R3 (240 GHz)	Retrievals down to 316 hPa
OzoneOnly	O_3, CO	R3 (240 GHz)	Retrievals down to 316 hPa
CorePlusR2	H_2O, N_2O, HNO_3, ClO, O_3, HCN, CH_3CN, SO_2, pTan (GHz)	R1A & R1B (118 GHz), R2 (190 GHz)	H_2O retrieved down to 316 hPa, other species 100 hPa (note no T, GPH retrieval)
Hydrogen Cyanide	HCN, O_3, HNO_3	R2 (190 GHz)	Retrievals down to 100 hPa
NitrousOxide	H_2O, N_2O	R2 (190 GHz)	Optimized to produce good N_2O product, retrievals down to 215 hPa
CorePlusR4AB14	ClO, BrO, HO_2, HOCl, HCl, O_3, HNO_3, CH_3CN, SO_2, CH_3Cl	R4 (640 GHz)	Retrievals down to 147 hPa
Methanol	CH_3OH, ClO, BrO, HO_2, HOCl, HNO_3, SO_2, CH_3Cl	R2 (190 GHz) and R4 (640 GHz)	Retrievals down to 147 hPa
CorePlusR4AB13	HCl, O_3, SO_2	R4 (640 GHz)	Retrievals down to 147 hPa. This phase only performed when MLS band 13 is operating
CorePlusR4B	N_2O, SO_2	R4 (640 GHz)	Retrievals down to 147 hPa
HighCloud	Cloud induced radiance, IWC, IWP	—	Used for flagging clouds in Core+R3 and later phases and forms basis for cloud ice products.
CorePlusR5	T, pTan (GHz, THz), GPH, OH, O_3	R1A & R1B (118 GHz), R5H and R5V (2.5 THz)	Retrievals down to 68 hPa (147 hPa for Temperature)
GPHOnly	GPH	—	Offsets CorePlusR3 GPH to match GEOS-5 at 100 hPa

[1]Tangent pressure and Geopotential height have been abbreviated to pTan (GHz/THz) and GPH respectively. Minor state vector components such as "baseline" and/or 'extinction' have been omitted unless they are the specific focus of the phase. Temperature, IWC, H_2O, RHi are "high resolution" (12 surfaces per decade change in pressure from 1000 hPa to 1 hPa) unless otherwise stated. O_3 is low resolution except for the Core+R3 phase.

[2]On high vertical resolution grid

Table 2.3.2: The origin of each of the “standard products” from v5.0x.

Product	Origin	Spectral region
BrO	`CorePlusR4AB14`	640 GHz
CH_3Cl	`CorePlusR4AB14`	640 GHz
CH_3CN	`CorePlusR4AB14`	640 GHz
CH_3OH	`Methanol`	640 GHz
ClO	`CorePlusR4AB14`	640 GHz
CO	`CorePlusR3`	240 GHz
GPH	`GPHOnly`	118 & 240 GHz
H_2O	`CorePlusR2`	190 GHz
HCl	`CorePlusR4AB14`	640 GHz
HCN	`HydrogenCyanide`	190 GHz
HNO_3	`CorePlusR2` (15 hPa and less) `CorePlusR3` (larger than 15 hPa)	190 GHz 240 GHz
HO_2	`CorePlusR4AB14`	640 GHz
HOCl	`CorePlusR4AB14`	640 GHz
IWC	`HighCloud`	240 GHz
IWP	`HighCloud`	240 GHz
N_2O	`NitrousOxide`	190 GHz
O_3	`OzoneOnly`	240 GHz
OH	`CorePlusR5`	2.5 THz
RHi	Computed from Temperature and H_2O	190 GHz
SO_2	`CorePlusR3`	240 GHz
Temperature	`CorePlusR3`	118 & 240 GHz

Table 2.5.1: MLS frequency channels and thresholds for cloud flag

Radiometer	Cloud channel	USB/LSB frequency / GHz	Low threshold	High threshold
R1[A/B]:118	B[32/34]W:PT.C4	115.3 (LSB only)	$T_{cir} < -4$ K	none
R2:190	B5F:ClO.C1	178.8 / 204.9	$T_{cir} < -20$ K	$T_{cir} > 10$ K
R3:240	B8F:PT	233.4–234.5 / 244.8–245.9	none	$\chi^2 > 30$
R4:640	B11F:BrO.C23	635.9 / 649.8	$T_{cir} < -10$ K	none

Cloud radiance scattering causes severe line shape distortions which are most reliably detectable in the Band 8 $O^{18}O$ line fit, based on extrapolating a tangent pressure estimate into the upper troposphere from the pressure information obtained from the 118 GHz Band 1 measurements (unaffected by clouds). RHi from a previous phase is used to compute a cloud induced radiance (T_{cir}). The vertical profiles of χ^2 and T_{cir} are analyzed to find the highest limb view affected by cloud scattering, and radiances below are handled accordingly.

The other aspect of cloud handling in v5.0*x* is the estimation of cloud ice water content (IWC) and ice water path (IWP) products from the final T_{cir} computed by the retrieval in the `HighCloud` phase. More information on these products and their derivation is given in Section 3.15.

2.6 The quantification of systematic uncertainty in MLS data

A major component of the validation of MLS data is the quantification of the various sources of systematic uncertainty. These can arise from instrumental issues (e.g., radiometric calibration, field of view characterization), spectroscopic uncertainty, and through approximations in the retrieval formulation and implementation. A comprehensive quantification of these uncertainties has been performed for the older v4.2*x* MLS products, updated from that described in the MLS validation papers (which were based on v2.2). The individual sections of Chapter 3 detail the results of this quantification product-by-product. We do not expect the estimated systematic errors in the MLS products to vary significantly between v5.0*x* and v4.2*x*; however, we do plan to update these estimates for v5.0*x* and report findings in an updated version of this document.

For each identified source of systematic uncertainty, its impact on MLS measurements of radiance (or pointing where appropriate) has been quantified and modeled. These modeled impacts correspond to either 2σ estimates of uncertainties in the relevant parameter(s), or an estimate of their maximum reasonable error(s) based on instrument knowledge and/or design requirements. Accordingly, the numbers reported for each product in Chapter 3 reflect 2σ estimates of potential systematic error.

For most of the uncertainty sources, the impact on MLS standard products has been quantified by running perturbed radiances through the MLS data processing algorithms. Other (typically smaller) uncertainty sources have been quantified by simple perturbation calculations.

Although the term "systematic uncertainty" is often associated with consistent biases and/or scaling errors, many sources of "systematic" error in the MLS measurement system give rise to additional scatter. For example, an error in the O_3 spectroscopy, while being a bias on the fundamental parameter, will have an impact on the retrievals of species with weaker signals (e.g., CO) that is dependent on the amount and morphology of atmospheric ozone. The extent to which such terms can be expected to average down is estimated to first order by these "full up studies" through their separate consideration of the bias and scatter each uncertainty source introduces.

The results of these studies are summarized as "accuracy" (and in some cases additional contributions to "precision") on a product by product basis in the next chapter. More details on the quantification for each product are given in the MLS validation papers. In addition Appendix A of *Read et al.* [2007] gives more specific details of the perturbations used in the study.

2.7 A brief note on the `Quality` field

As described in Section 1.6, the `Quality` field in the `L2GP` files gives a measure of the fit achieved between the observed MLS radiances and those computed by the forward model given the retrieved MLS profiles. `Quality` is computed from a χ^2 statistic for all the radiances considered to have significantly affected the retrieved species (i.e., those close to the relevant spectral lines), normalized by dividing by the number of radiances. `Quality` is simply the reciprocal of this statistic (i.e., low values indicate large χ^2, i.e., poor fits).

Ideally, the typical values of these normalized χ^2 statistics will be around one, indicating that radiances are typically fitted to around their noise levels. `Quality` will therefore also ideally have a typical value of one. For some species, however, because of uncertain knowledge of spectroscopy and/or instrument calibration, the v5.0*x* algorithms are known to be consistently unable to fit some observed radiances to within their predicted noise. In many of these cases, the noise reported on the radiances has been "inflated" to allow the retrieval more leeway in fitting to radiances known to be challenging. As the noise level is the denominator in the χ^2 statistic, these species will have typical χ^2 statistics that are less than one and thus typical values of `Quality` higher than one. Accordingly, differences in `Quality` from one species to another do not reflect the species' relative validity, nor do version-to-version increases in `Quality` for a given product necessarily indicate improvements (or vice versa)

Chapter 3
Product-specific information

3.1 Overview of species-specific discussion

This section describes each MLS v5.0*x* "standard product" in more detail. An overview is given of the expected resolution, precision and accuracy of the data. The resolution is characterized by the averaging kernels described below. Precision is quantified through a combination of the precision estimated by the MLS v5.0*x* algorithms, through reference to the systematic uncertainty budget described in section 2.6, and through study of the actual MLS data (e.g., consideration of the observed scatter in regions where little natural variability is anticipated).

The systematic uncertainty reported is generally based on the study described in section 2.6. However, in some cases larger disagreements are seen between MLS and correlative observations than these quantifications would imply. In such cases (e.g., MLS 215 hPa CO) the uncertainty quoted reflects these disagreements.

A note on the averaging kernel plots

The averaging kernels shown in this section describe both the horizontal (along track) and vertical (pressure) resolution of the MLS v5.0*x* data. While the averaging kernels vary somewhat from profile to profile, their variation is sufficiently small that these samples can be considered representative for all profiles. The averaging kernel plots are accompanied by estimates of the horizontal and vertical resolution of the product defined by the full width at half maximum of the kernels. Each kernel plot also shows the integrated areas under the kernels.

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3.2 Bromine monoxide (BrO)

Swath name: `BrO`

Useful range: 10–3.2 hPa (day/night differences needed)

Contact: Luis Millán, **Email:** <Luis.F.Millan@jpl.nasa.gov>

3.2.1 Introduction

The standard product for BrO is taken from the 640-GHz `CoreR4AB14` retrieval. The spectral signature of BrO in the MLS radiances is very small, leading to a very poor signal-to-noise ratio on individual MLS observations. Significant averaging (e.g., monthly zonal means) is required to obtain scientifically useful results. Large biases of between 12 to 43 pptv (typical BrO abundances range from 5 to 15 pptv) are seen in the data. These biases can be minimized by taking day/night differences. For pressures of 4.6 hPa and greater, nighttime BrO is negligible; however, for smaller pressures, nighttime BrO needs to be taken into account. Table 3.2.1 summarizes the precision, accuracy, and resolution of the MLS v5.0*x* BrO product. The accuracy assessment is based on v2.2 data, as described in the validation paper [*Kovalenko et al.*, 2007].

Note, the v5.0*x* "standard" BrO product (as with earlier versions) contains systematic biases and horizontal oscillations that present a larger challenge than for other species. Those interested in using MLS BrO in scientific studies are strongly advised to contact the MLS team before embarking on their research. Different algorithms for BrO have been developed by the MLS team, aimed at ameliorating some of these artifacts [*Millán et al.*, 2012], and those products are available from the GSFC DISC. The product short name is "`ML3DZMBRO`" and it is available from: `https://disc.gsfc.nasa.gov/datacollection/ML3DZMBRO_004.html`.

3.2.2 Vertical Resolution

Figure 3.2.1 shows that the vertical resolution for the v5.0*x* MLS BrO is about 5.5 km in the 10 to 4.6 hPa pressure region, degrading to 6 km at 3.2 hPa.

3.2.3 Precision

The expected precision in a retrieved profile is calculated from radiance noise and reported for each retrieved data point. The value of the expected precision is flagged negative or zero if it is worse than 50% of the value of the a priori precision. Figure 3.2.2 compares the expected precision (thick line) on an individual MLS BrO measurement with that deduced from observations of scatter in night-time observations (expected to be zero). Also shown are the expected precisions for daily, monthly, and yearly 10° zonal means. For the minimal averaging recommended, a monthly 10° zonal mean, which corresponds to about 3,000 measurements, the precision is about ±4 ppt. See Table 3.2.1 for more details.

3.2.4 Accuracy

The accuracy of the MLS BrO product is summarized in Table 3.2.1. The effect of each identified source of systematic error on MLS measurements of radiance has been quantified and modeled [*Read et al.*, 2007]. These quantified effects correspond to either 2σ estimates of uncertainties in each MLS product, or an estimate of the maximum reasonable uncertainty based on instrument knowledge and/or design requirements. More discussion is given in *Kovalenko et al.* [2007]. While that paper described v2.2 BrO, findings are expected to be applicable also to v5.0*x*. The potential systematic bias in MLS BrO measurements can be as high as about ±43 ppt at 10 hPa, decreasing to about ±12 pptv at 3.2 hPa. The

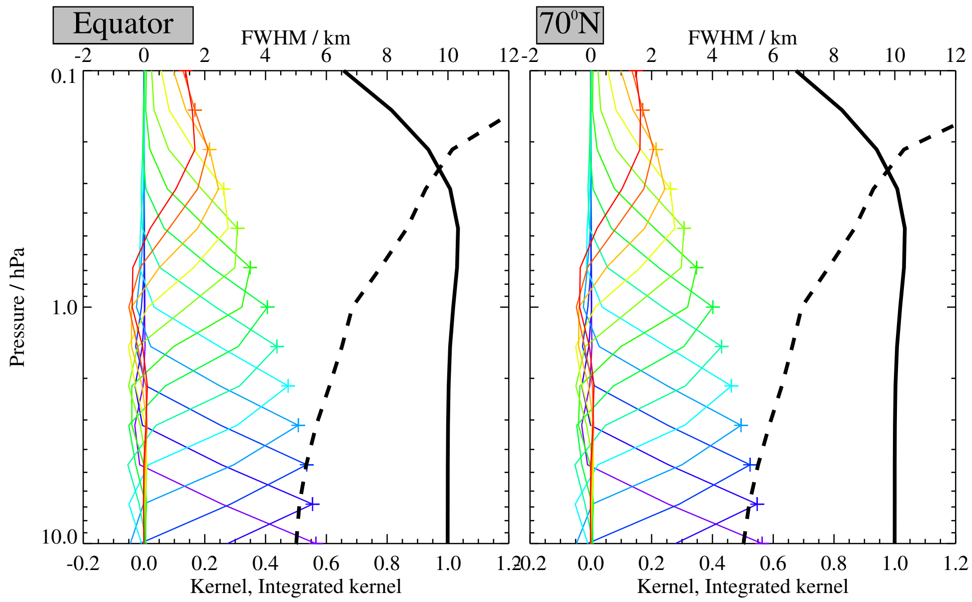

Figure 3.2.1: Typical vertical averaging kernels for the MLS v5.0x BrO data at the equator (left) and at 70°N (right); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the vertical resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). The solid black line shows the integrated area under each kernel; values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. The low signal to noise for this product necessitates the use of significant averaging (e.g., monthly zonal mean), making horizontal averaging kernels largely irrelevant.

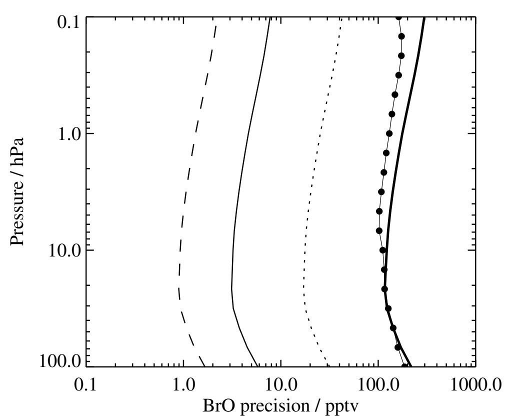

Figure 3.2.2: Comparison of the MLS v5.0x BrO precision as estimated from scatter in the retrieved data (circles) with that expected from the retrieval (thick line), for a single profile. Also shown is the expected precision for the day/night difference of 10° zonal mean profiles averaged over a day (dotted line), a month (thin line) and a year (dashed line).

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

systematic bias is dramatically reduced by subtracting the nighttime signal from the daytime signal. Taking the day/night difference reduces the systematic biases to ±16 pptv at 10 hPa and to ±9 pptv at 3.2 hPa. If the MLS BrO data is used at 3.2 hPa, the day/night difference value will need to be adjusted to compensate for the non-negligible nighttime BrO. We note that this method of taking day/night differences is not applicable for polar summer and winter during periods of continuous sunlight or darkness.

3.2.5 Data screening

Pressure range: 10–3.2 hPa

Values outside this range are not recommended for scientific use.

Averaging required: Significant averaging (such as monthly zonal means) is required if useful scientific data are sought.

Diurnal differences: For use in any scientific study, day / night or ascending / descending differences should be used to alleviate biases.

Note that, for 3.2 hPa, the non-zero nighttime expected abundances BrO needs to be taken into account.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Clouds: Profiles identified as being affected by clouds can be used with no restriction.

Quality: Only profiles whose `Quality` field is greater than 1.3 should be used.

Convergence: Only profiles whose `Convergence` field is less than 1.05 should be used.

3.2.6 Artifacts

Significant biases exist in the BrO data, as discussed above. Day / night (or ascending / descending) differences must be used to reduce these. For 3.2 hPa, nighttime BrO needs to be taken into account [*Kovalenko et al.*, 2007].

A systematic horizontal (i.e., profile-to-profile) oscillation has been discovered in MLS v5.0*x* (and earlier) standard BrO product. This presents a significant challenge to the interpretation of the BrO observations. Users are strongly advised to contact the MLS team before embarking on research involving the MLS standard BrO product. As described above, use of other BrO products is preferable to using the Level 2 BrO data.

3.2.7 Review of comparisons with other data sets

We have calculated total bromine, Br_y, from MLS measurements of BrO using a photochemical model, and compared this with Br_y similarly inferred from balloon-borne measurements of BrO; good agreement is seen [*Kovalenko et al.*, 2007].

Table 3.2.1: Summary of the Aura MLS v5.0x BrO product.

Pressure range	Vertical res. / km	Precision[a] / pptv	Day/night difference accuracy[b] / pptv	Comments
2.2 hPa and less	–	–	–	Unsuitable for scientific use
3.2 hPa	6	±5	±8	Need to account for non-negligible night time BrO
4.6	5.5	±4	±10	
6.8	5.5	±4	±11	
10	5.5	±4	±13	
150–15 hPa	–	–	–	Unsuitable for scientific use
1000–215 hPa	–	–	–	Not retrieved

[a]The precision quoted is for a 10° monthly zonal mean

[b]Because of large biases in the data, the daytime and nighttime BrO data are unsuitable for scientific use, so day/night differences must be used. Note that day/night differences are not useful for polar winter and summer, where BrO does not undergo a diurnal variation.

3.3 Methyl chloride (CH_3Cl)

Swath name: `CH3Cl`

Useful range: 147–4.6 hPa

Contact: Michelle Santee, **Email:** <Michelle.L.Santee@jpl.nasa.gov>

3.3.1 Introduction

The v2.2 MLS ClO measurements were characterized by a substantial (∼0.1–0.4 ppbv) negative bias at retrieval levels below (i.e., pressures larger than) 22 hPa. *Santee et al.* [2008] suggested that contamination from an interfering species such as CH_3Cl, which has lines in two wing channels of the 640-GHz band used to measure ClO, could have given rise to the bias; they showed results from precursory v3 algorithms in which CH_3Cl was also retrieved that demonstrated significant reduction in the bias in lower stratospheric ClO. Further refinements in the v3.3*x*/v3.4*x* algorithms yielded not only an improved ClO product, but also a reliable retrieval of CH_3Cl. The quality and reliability of the v3.3*x*/v3.4*x* MLS CH_3Cl measurements were assessed in detail by *Santee et al.* [2013].

As is the case for ClO, the standard CH_3Cl product is derived from radiances measured by the radiometer centered near 640 GHz. The MLS v5.0*x* CH_3Cl data are scientifically useful over the range 147 to 4.6 hPa. A summary of the estimated precision, resolution (vertical and horizontal), and systematic uncertainty of the v5.0*x* CH_3Cl measurements as a function of altitude is given in Table 3.3.1.

3.3.2 Differences between v4.2*x* and v5.0*x*

As with other species retrieved from the MLS 640-GHz receiver, lower stratospheric signals for CH_3Cl are affected by water vapor. Therefore, for the retrieval phase CorePlusR4AB14, which includes CH_3Cl (see Table 2.3.1), water vapor is constrained to the values from the MLS H_2O standard product. As discussed in Section 3.9.2, the dry bias below the tropopause present in earlier MLS data versions has been mitigated in v5.0*x*. Some of the differences between v5.0*x* and v4.2*x* CH_3Cl can thus be attributed to the improvement in H_2O between the two versions. CH_3Cl abundances are uniformly larger in v5.0*x* than in v4.2*x* at the lowest retrieval levels (68–147 hPa). Low-latitude differences are generally in the range of 10–20% or less, whereas differences in the Southern Hemisphere polar region typically exceed 30% during austral summer and those in the Northern Hemisphere polar region typically exceed 20% during boreal summer (Figure 3.3.1). In addition, v5.0*x* mixing ratios are typically larger than those in v4.2*x* in the polar lower stratosphere in both hemispheres during their respective winter seasons, with differences of more than 30% in the Arctic (less in the Antarctic). In contrast, v5.0*x* abundances are smaller than those in v4.2*x* almost everywhere at higher altitudes (˜10 hPa and lower pressures). In general, the zonal-mean CH_3Cl distribution (at all latitudes) is smoother and more realistic in v5.0*x* (Figure 3.3.1), although the overall systematic uncertainty at 147 hPa has increased (see Section 3.3.6).

3.3.3 Resolution

The resolution of the retrieved data can be described using "averaging kernels" [e.g., *Rodgers*, 2000]; the two-dimensional nature of the MLS data processing system means that the kernels describe both vertical and horizontal resolution. Values of the integrated kernel near unity indicate that the majority of information for that level has come from the measurements themselves and not the a priori; Figure 3.3.2 shows that the measurements dominate at pressures greater than 3.2 hPa, above which level the integrated kernel drops below 0.5. Smoothing, imposed on the retrieval system in both the vertical and horizontal directions to enhance retrieval stability and precision, degrades the inherent resolution of the measurements. Thus, although CH_3Cl measurements are reported at six pressure levels per decade

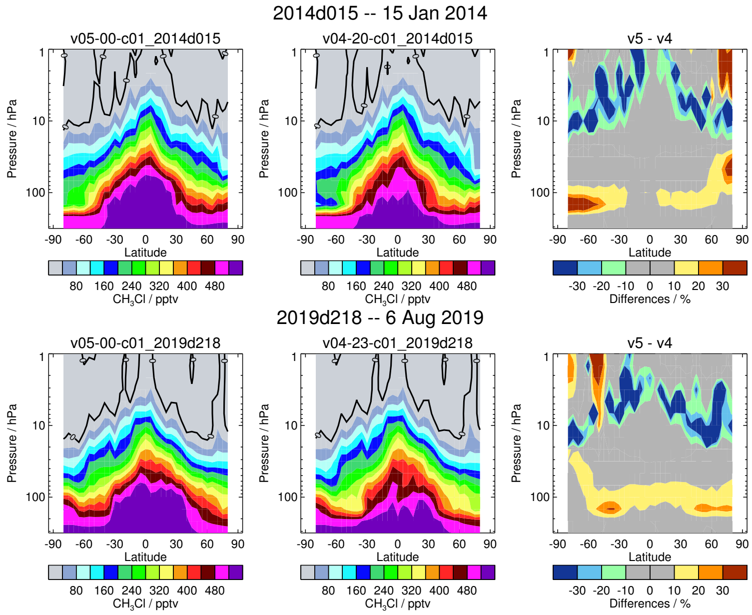

Figure 3.3.1: Zonal mean pressure-latitude cross sections of MLS CH_3Cl, for (left) v5.0x, (middle) v4.2x, and (right) their differences (v5.0x minus v4.2x, in percent). Results are shown for representative days during summer in each hemisphere. The black curves overlaid on the abundance panels (left and middle) mark the zero contour.

change in pressure (spacing of ∼2.7 km), the vertical resolution of the v5.0*x* CH_3Cl data as determined from the full width at half maximum of the rows of the averaging kernel matrix shown in Figure 3.3.2 is ∼4–6 km in most of the lower stratosphere, degrading to ∼8–10 km at and above (i.e., at pressures less than) 15 hPa. The averaging kernels are fairly symmetric, and for the most part they peak at their nominal position. However, overlap in the averaging kernels for the 100 and 147 hPa retrieval surfaces indicates that the 147 hPa retrieval does not provide as much independent information as is given by retrievals at higher altitudes. Figure 3.3.2 also shows horizontal averaging kernels, from which the along-track horizontal resolution is determined to be ∼600 km at 147 hPa, ∼450–500 km from 100 to 22 hPa, and ∼600–850 km at and above 15 hPa. The cross-track resolution, set by the width of the field of view of the 640-GHz radiometer, is ∼3 km. The along-track separation between adjacent retrieved profiles is 1.5° great circle angle (∼165 km), whereas the longitudinal separation of MLS measurements, set by the Aura orbit, is 10°–20° over low and middle latitudes, with much finer sampling in the polar regions.

3.3.4 Precision

The precision of the MLS CH_3Cl data is estimated empirically by comparing profiles measured at the intersections of ascending (mainly day) and descending (mainly night) portions of the orbit. Under ideal conditions (i.e., a quiescent atmosphere), the standard deviation about the mean differences between such matched profile pairs provides a measure of the precision of the individual data points. In practice, however, real changes in the atmosphere may occur over the 12 h interval between the intersecting measurement points, in which case the observed scatter provides an upper limit on the estimate of precision, assuming that the a priori has a negligible influence on the retrieval (a reasonable assumption at least at pressures greater than 3.2 hPa). The precision estimates were found to be essentially invariant with time; results for several months of a representative year of data are shown in Figure 3.3.3. The observed

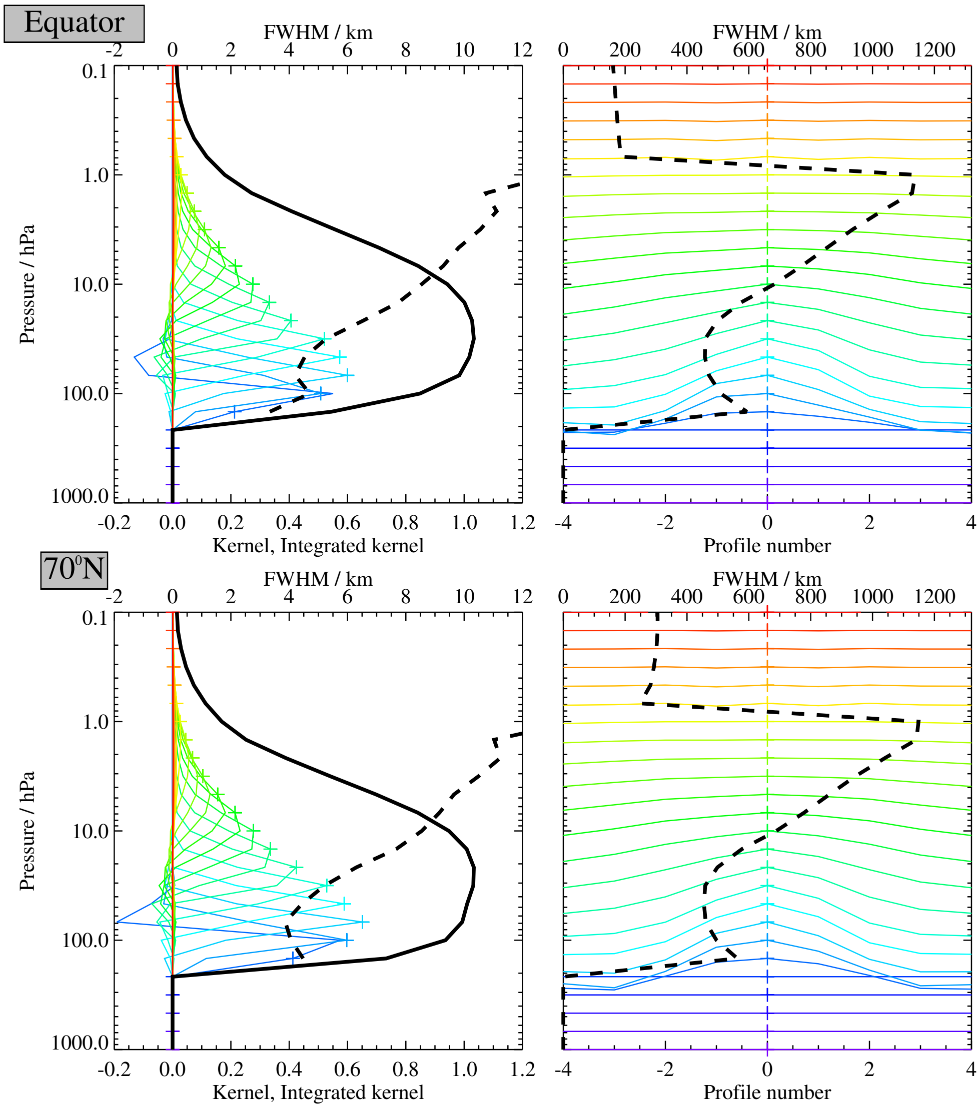

Figure 3.3.2: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x CH_3Cl data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

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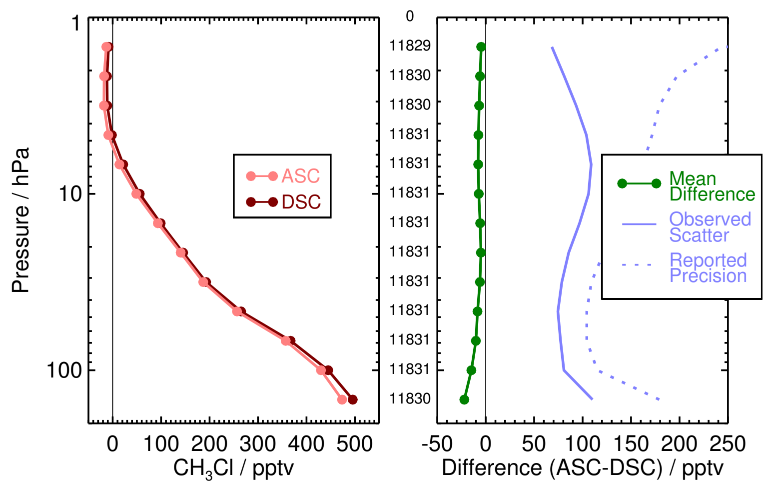

Figure 3.3.3: (left) Ensemble mean profiles for ascending (light red) and descending (dark red) orbit matching pairs of MLS v5.0x CH_3Cl profiles averaged over several months of a representative year of data (2009). Symbols indicate MLS retrieval pressure levels. (right) Mean differences (ascending—descending) in pptv (green solid line). Also shown are the standard deviations about the mean differences (light blue solid line) and the root sum square (RSS) of the precisions calculated by the retrieval algorithm for the two sets of profiles (light blue dotted line). The observed scatter about the mean differences and the reported precision values have been scaled by $1/\sqrt{2}$ (to convert from standard deviations of differences into standard deviations of individual data points); hence the light blue solid line represents the statistical repeatability of the MLS measurements, and the light blue dotted line represents the expected 1σ precision for a single profile. The thin black lines mark zero in each panel. The number of crossing pairs of measurements being compared at each pressure level is noted in the space between the panels.

standard deviation values are ~100 pptv or less throughout the vertical domain. Mean differences between paired crossing profiles are ~10 pptv or less except at the lowest two levels, where they reach ~15–25 pptv. Given the large number of data points being compared, these ascending–descending differences are substantially larger than the standard error of the mean, implying the presence of significant systematic biases. These biases likely arise from the cumulative effect of various factors in the retrieval system that can vary diurnally or along the orbit, such as interferences from temperature or other atmospheric constituents (e.g., H_2O and ClO), or thermal emissions from the MLS antenna.

The precision reported for each data point by the Level 2 data processing system exceeds the observationally determined precision throughout the vertical range (Figure 3.3.3), indicating that the vertical smoothing (regularization) applied to stabilize the retrieval system and improve the precision has a non-negligible influence. Because the reported precisions take into account occasional variations in instrument performance, the best estimate of the precision of an individual data point is the value quoted for that point in the L2GP files, but it should be borne in mind that this approach slightly overestimates the actual measurement noise. The estimates reported here represent the precisions at each pressure level of a single profile; precision can generally be improved by averaging, with the precision of an average of N profiles being $1/\sqrt{N}$ times the precision of an individual profile (although the actual standard error of the mean can in some cases be even smaller [*Toohey and von Clarmann*, 2013]).

3.3.5 Range

Although CH_3Cl is retrieved over the range 147 to 0.001 hPa, because of the degradation in resolution and expected precision, the reduction in independent information contributed by the measurements, and the results of simulations using synthetic data as input radiances to test the closure of the retrieval system, the data are not deemed reliable at retrieval pressures less than 4.6 hPa. Despite the overlap in the averaging kernels for the 147 and 100 hPa surfaces discussed above, the simulations show that the retrieved CH_3Cl values track the variations in the “truth” field at both levels. Moreover, the retrievals (of real data) at 147 hPa display significant features not seen at 100 hPa (not shown) that are believed to represent actual atmospheric variations. Thus, we recommend that the v5.0*x* CH_3Cl data may be used for scientific studies between 147 and 4.6 hPa (inclusive), although the reduced sensitivity at the extremes of this range, as well as the relatively coarse vertical resolution of the retrieved profiles, should be borne in mind.

3.3.6 Accuracy

The effects of various sources of systematic uncertainty (e.g., instrumental issues, spectroscopic uncertainty, and approximations in the retrieval formulation and implementation) on the MLS v5.0*x* CH_3Cl measurements have been quantified through a comprehensive set of retrievals of synthetic radiances; see *Santee et al.* [2013] for details of a similar analysis conducted on MLS v3.3*x*/v3.4*x* CH_3Cl data. The overall systematic uncertainty, or accuracy, is calculated by combining (RSS) the contributions from both the expected biases and the additional scatter each source of uncertainty may introduce into the data. In aggregate, the factors considered in these simulations are estimated to give rise to total systematic uncertainty of approximately 25–65% in the MLS v5.0*x* CH_3Cl data in the upper troposphere / lower stratosphere (see Table 3.3.1). These values for the overall uncertainty in v5.0*x* CH_3Cl are slightly smaller (better accuracy) than those estimated for the v4.2*x* data [see *Livesey et al.*, 2020] at the top of the recommended range but slightly larger (poorer accuracy) at 147 hPa.

3.3.7 Review of comparisons with other datasets

Extensive comparisons of MLS v3.3*x*/v3.4*x* CH_3Cl data with a variety of different platforms (balloon-borne, aircraft, and satellite instruments) were presented by *Santee et al.* [2013]. Comparisons of v5.0*x* CH_3Cl with correlative data have not been conducted but are expected to yield results similar to those for previous versions.

3.3.8 Data screening

Pressure range: 147–4.6 hPa

Values outside this range are not recommended for scientific use.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is zero.

We recommend that all profiles with nonzero values of `Status` be discarded, because of the potential impact of cloud artifacts at lower levels. Note, however, that rejecting in their entirety all profiles with nonzero `Status` may be unnecessarily severe at and above (i.e., at pressures equal to or smaller than) 46 hPa, where clouds have negligible impact; thus otherwise good-quality profiles with nonzero but even `Status` values may be used without restriction at those levels as long as they are removed at larger pressures. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality: Only profiles whose `Quality` field is greater than 1.3 should be used.

This threshold for `Quality` (unchanged from v4.2*x*) typically excludes less than 1% of CH_3Cl profiles on a daily basis; note that it potentially discards some "good" data points while not necessarily identifying all "bad" ones.

Convergence: Only profiles whose `Convergence` field is less than 1.05 should be used.

On a typical day this threshold for `Convergence` (unchanged from v4.2*x*) discards few (0.5% or less) of the CH_3Cl profiles, most (but not all) of which are also filtered out by the other quality control measures.

3.3.9 Artifacts

- Significant ascending—descending differences imply the presence of systematic biases at the bottom two retrieval pressure levels. However, various analyses performed separately on sets of ascending-only and descending-only measurements suggest that, although significant, these biases will have little or no impact on most scientific conclusions based on the MLS CH_3Cl measurements.

3.3.10 Desired improvements for future data version(s)

- Minimize the impact of thick clouds on the retrievals to further improve the CH_3Cl measurements in the upper troposphere and lowermost stratosphere.

Table 3.3.1: Summary of Aura MLS v5.0x CH_3Cl Characteristics

Pressure / hPa	Resolution V × H[a] / km	Precision[b] / pptv	Systematic Uncertainty[c] / %	Known Artifacts or Other Comments
3.2–0.001	—	—	—	Unsuitable for scientific use
15–4.6	8–10 × 600–850	±100	±25–65	
100–22	4–6.5 × 450–500	±100	±35–50	
147	4 × 600	±100	±65	
1000–215	—	—	—	Not retrieved

[a] Vertical and Horizontal resolution in along-track direction.
[b] Precision on individual profiles.
[c] Values should be interpreted as 2-σ estimates of the probable magnitude.

3.4 Methyl cyanide (CH_3CN)

Swath name: `CH3CN`

Useful range: 46–1.0 hPa

Contact: Michelle Santee, **Email:** <Michelle.L.Santee@jpl.nasa.gov>

3.4.1 Introduction

In v5.0*x*, as in v4.2*x*, the standard CH_3CN product is taken from radiances measured by the radiometer centered near 640 GHz. The CH_3CN retrieval is largely unchanged in v5.0*x*. Although the data have not been validated extensively, the v5.0*x* CH_3CN retrievals are deemed to be scientifically useful over the range 46 to 1 hPa, except in the winter polar regions, where they may exhibit large biases below (i.e., at pressures higher than) 10 hPa. Data retrieved at higher pressures may be used with caution in certain circumstances. A summary of the estimated precision, resolution (vertical and horizontal), and systematic uncertainty of the v5.0*x* CH_3CN measurements as a function of altitude is given in Table 3.4.1.

3.4.2 Differences between v4.2*x* and v5.0*x*

Except at the top end of the retrieval range (where the data are generally of less interest), the CH_3CN retrieval is little changed between v4.2*x* and v5.0*x*, with differences less than 10% in most regions (Figure 3.4.1). Larger (20–30%, both positive and negative) differences are occasionally seen in the winter polar lower stratosphere in both hemispheres, where the data are known to be biased.

3.4.3 Resolution

The resolution of the retrieved data can be described using "averaging kernels" [e.g., *Rodgers*, 2000]; the two-dimensional nature of the MLS data processing system means that the kernels describe both vertical and horizontal resolution. Values of the integrated kernel near unity indicate that the majority of information for that level has come from the measurements themselves and not the a priori; Figure 3.4.2 shows that the measurements dominate throughout most of the vertical range. Smoothing, imposed on the retrieval system in both the vertical and horizontal directions to enhance retrieval stability and precision, degrades the inherent resolution of the measurements. Thus, although CH_3CN measurements are reported at six pressure levels per decade change in pressure (spacing of ∼2.7 km), the vertical resolution of the v5.0*x* CH_3CN data as determined from the full width at half maximum of the rows of the averaging kernel matrix shown in Figure 3.4.2 degrades from 4.5 km at 147 hPa to ∼5–6.5 km in the lower stratosphere, and then further worsens to ∼7–8 km in the upper stratosphere. Substantial overlap in the averaging kernels for the 100 and 147 hPa retrieval surfaces (which both peak at 100 hPa) indicates that the 147 hPa retrieval does not provide as much independent information as is given by retrievals at higher altitudes. Figure 3.4.2 also shows horizontal averaging kernels, from which the along-track horizontal resolution is determined to be ∼400–700 km over most of the vertical range. The cross-track resolution, set by the width of the field of view of the 640-GHz radiometer, is ∼3 km. The along-track separation between adjacent retrieved profiles is 1.5° great circle angle (∼165 km), whereas the longitudinal separation of MLS measurements, set by the Aura orbit, is 10°–20° over low and middle latitudes, with much finer sampling in the polar regions.

3.4.4 Precision

The precision of the MLS CH_3CN data is estimated empirically by comparing profiles measured at the intersections of ascending (mainly day) and descending (mainly night) portions of the orbit. Under ideal conditions (i.e., a quiescent atmosphere), the standard deviation about the mean differences between such matched profile pairs provides a measure of the precision of the individual data points. In

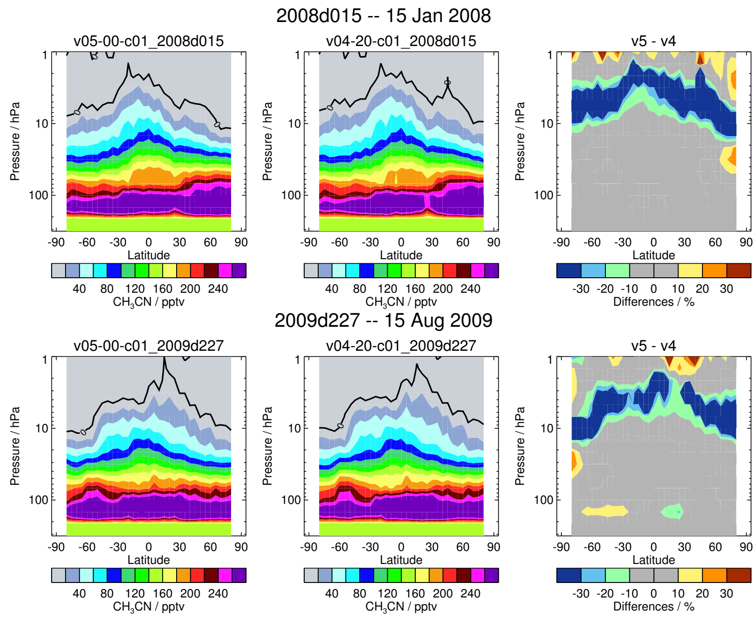

Figure 3.4.1: Zonal mean pressure-latitude cross sections of MLS CH_3CN, for (left) v5.0x, (middle) v4.2x, and (right) their differences (v5.0x minus v4.2x, in percent). Results are shown for representative days during winter in each hemisphere. The black curves overlaid on the abundance panels (left and middle) mark the zero contour.

practice, however, real changes in the atmosphere may occur over the 12 h interval between the intersecting measurement points, in which case the observed scatter provides an upper limit on the estimate of precision, assuming that the a priori has a negligible influence on the retrieval (a reasonable assumption throughout the retrieval range for CH_3CN). The precision estimates were found to be essentially invariant with time; results for several months of a representative year of data are shown in Figure 3.4.3. Mean differences between paired crossing profiles are negligible, indicating the absence of significant systematic ascending / descending biases. The observed standard deviation values are ~50 pptv or less throughout most of the vertical domain, increasing to 100 pptv at 147 and 1 hPa.

The precision reported for each data point by the Level 2 data processing system exceeds the observationally determined precision throughout the vertical range (Figure 3.4.3), indicating that the vertical smoothing (regularization) applied to stabilize the retrieval system and improve the precision has a non-negligible influence. Because the reported precisions take into account occasional variations in instrument performance, the best estimate of the precision of an individual data point is the value quoted for that point in the L2GP files, but it should be borne in mind that this approach slightly overestimates the actual measurement noise. The estimates reported here represent the precisions at each pressure level of a single profile; precision can generally be improved by averaging, with the precision of an average of N profiles being $1/\sqrt{N}$ times the precision of an individual profile (although the actual standard error of the mean can in some cases be even smaller [*Toohey and von Clarmann*, 2013]).

3.4.5 Range

Although CH_3CN is retrieved (and reported in the L2GP files) over the range 147 to 0.001 hPa, on the basis of the drop off in precision and resolution, the lack of independent information contributed by the measurements, and the results of simulations using synthetic data as input radiances to test the closure of the retrieval system, the data are not deemed reliable at the extremes of the retrieval range. Thus we recommend that v5.0*x* CH_3CN be used for scientific studies only at the levels between

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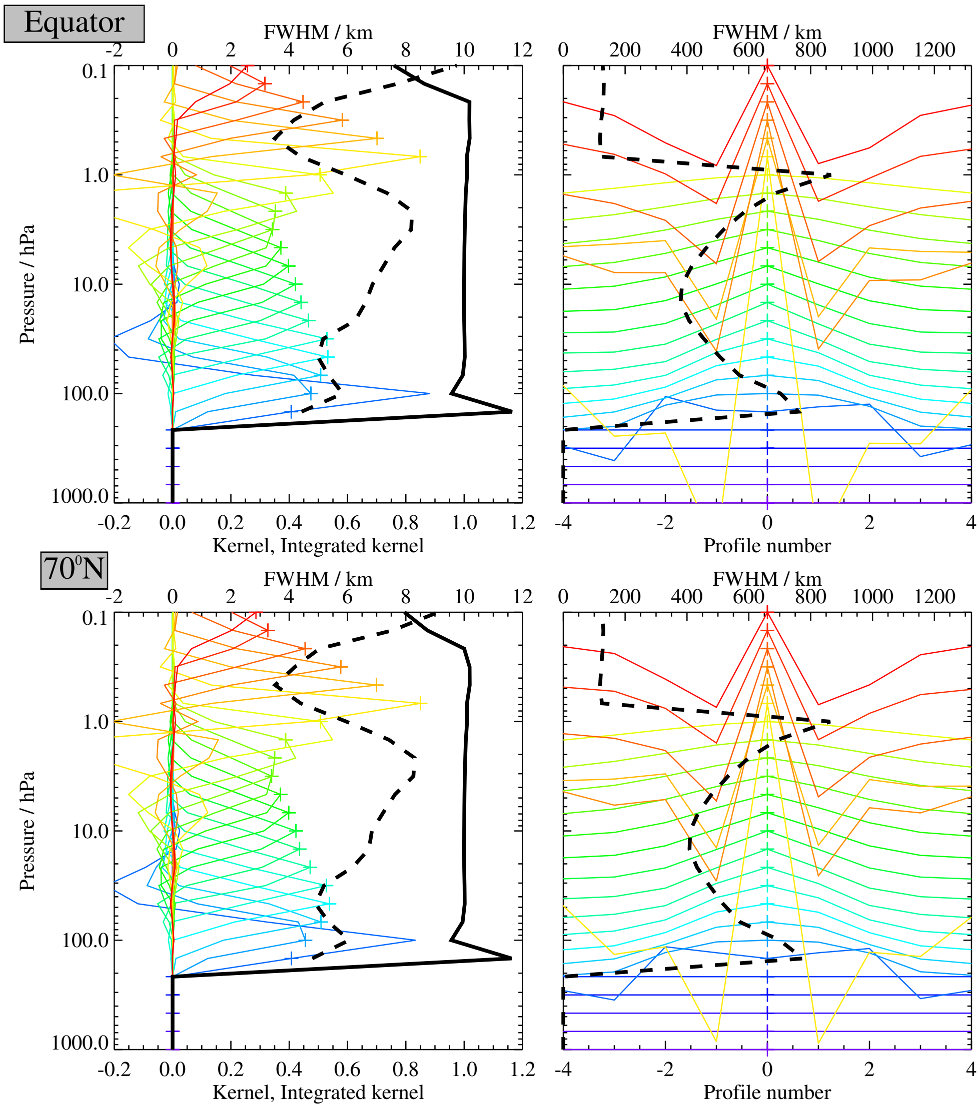

Figure 3.4.2: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x CH_3CN data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

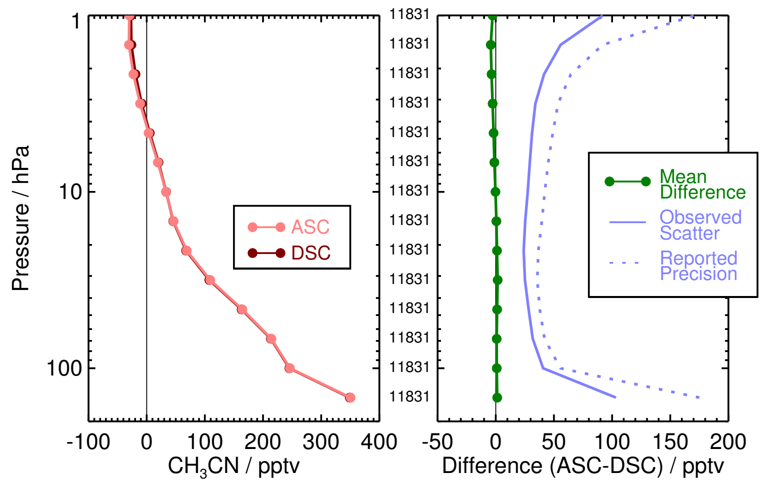

Figure 3.4.3: (left) Ensemble mean profiles for ascending (light red) and descending (dark red) orbit matching pairs of MLS v5.0x CH_3CN profiles averaged over several months of a representative year of data (2009). Symbols indicate MLS retrieval pressure levels. (right) Mean differences (ascending—descending) in pptv (green solid line). Also shown are the standard deviations about the mean differences (light blue solid line) and the root sum square (RSS) of the precisions calculated by the retrieval algorithm for the two sets of profiles (light blue dotted line). The observed scatter about the mean differences and the reported precision values have been scaled by $1/\sqrt{2}$ (to convert from standard deviations of differences into standard deviations of individual data points); hence the light blue solid line represents the statistical repeatability of the MLS measurements, and the light blue dotted line represents the expected 1σ precision for a single profile. The thin black lines mark zero in each panel. The number of crossing pairs of measurements being compared at each pressure level is noted in the space between the panels.

46 and 1 hPa, except in the winter polar regions, where they may exhibit large biases below 10 hPa. However, although the 147, 100, and 68 hPa retrievals are not generally recommended, they may be scientifically useful in some circumstances. For example, the data display unphysical sharp latitudinal gradients at ±30° at 100 and 68 hPa, yet the large-scale longitudinal variations within the tropics are probably robust. Similarly, confined regions of significant enhancement at 147 hPa unaccompanied by comparably enhanced values at 100 hPa may reflect real atmospheric features. Indeed, many of the “hotspots” apparent in MLS CH_3CN measurements in the upper troposphere / lower stratosphere (UTLS) closely track similar enhancements in other pollution markers measured by MLS, such as CO and CH_3Cl. The v5.0*x* CH_3CN data at the lowest retrieval levels (147–68 hPa) should only be used in consultation with the MLS science team.

3.4.6 Accuracy

The effects of various sources of systematic uncertainty (e.g., instrumental issues, spectroscopic uncertainty, and approximations in the retrieval formulation and implementation) on the MLS v5.0*x* CH_3CN measurements have been quantified through a comprehensive set of retrievals of synthetic radiances. The overall systematic uncertainty, or accuracy, is calculated by combining (RSS) the contributions from both the expected biases and the additional scatter each source of uncertainty may introduce into the data. In aggregate, the factors considered in these simulations are estimated to give rise to total systematic uncertainty of approximately 60–200% in the MLS v5.0*x* CH_3CN data (see Table 3.4.1).

3.4.7 Review of comparisons with other datasets

Detailed quantification of differences from correlative data sets has not been performed, but preliminary comparisons suggest that the MLS CH_3CN measurements are biased substantially high in the UTLS relative to airborne [*Singh et al.*, 2003], balloon-borne [*Kleinböhl et al.*, 2005], and ACE-FTS satellite [*Harrison and Bernath*, 2013] CH_3CN measurements, as do results from a two-dimensional chemistry transport model and (noncoincident) CH_3CN retrievals from the predecessor MLS instrument on the Upper Atmosphere Research Satellite (UARS) [*Livesey et al.*, 2001] (not shown). Furthermore, the zonal-mean morphology of the Aura MLS CH_3CN at the lowest levels does not agree well with that either observed by UARS MLS or predicted by the model.

3.4.8 Data screening

Pressure range: 46–1.0 hPa

Values outside this range are not recommended for scientific use. The CH_3CN data at 147–68 hPa may be useful under certain circumstances but should not be analyzed in scientific studies without significant discussion with the MLS science team.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is zero.

We recommend that all profiles with nonzero values of `Status` be discarded, because of the potential impact of cloud artifacts at lower levels. Note, however, that rejecting in their entirety all profiles with nonzero `Status` may be unnecessarily severe at and above (i.e., at pressures equal to or smaller than) 46 hPa, where clouds have negligible impact; thus otherwise good-quality profiles with nonzero but even `Status` values may be used without restriction at those levels as long as they are removed at larger pressures. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality: Only profiles whose `Quality` field is greater than 1.4 should be used.

This threshold for `Quality` (unchanged from v4.2*x*) typically excludes few (less than 0.5%) CH_3CN profiles on a daily basis; note that it potentially discards some "good" data points while not necessarily identifying all "bad" ones.

Convergence: Only profiles whose `Convergence` field is less than 1.05 should be used.

On a typical day this threshold for `Convergence` (unchanged from v4.2*x*) discards few (0.5% or less) of the CH_3CN profiles, many (but not all) of which are filtered out by the other quality control measures.

3.4.9 Artifacts

- The retrievals at 100 and 68 hPa are characterized by unphysical sharp latitudinal gradients at ±30°.
- Substantial biases may be present in the mixing ratios in the winter polar regions for retrieval levels in the range 100–15 hPa.

3.4.10 Desired improvements for future data version(s)

- Specific achievable improvements in the CH_3CN retrieval remain to be determined.

Table 3.4.1: Summary of Aura MLS v5.0x CH_3CN Characteristics

Pressure / hPa	Resolution V × H[a] / km	Precision[b] / pptv	Systematic Uncertainty[c] / %	Known Artifacts or Other Comments
0.68–0.001	—	—	—	Unsuitable for scientific use
1.0	6 × 850	±100	±160	Consult with MLS science team
10–1.5	7–8 × 400–700	±50	±100–160	Consult with MLS science team
46–15	5–6.5 × 400–500	±50	±100–160	Consult with MLS science team
100–68	5.5 × 550–700	±50	±60–100	Consult with MLS science team
147	4.5 × 750	±100	±200	Consult with MLS science team
1000–215	—	—	—	Not retrieved

[a]Vertical and Horizontal resolution in along-track direction.
[b]Precision on individual profiles.
[c]Values should be interpreted as 2-σ estimates of the probable magnitude.

3.5 Methanol (CH_3OH)

Swath name: `CH3OH`

Useful range: Contact the MLS science team before contemplating use (only useful over 147–100 hPa, with caution).

Contact: Michelle Santee, **Email:** <Michelle.L.Santee@jpl.nasa.gov>

3.5.1 Introduction

The standard CH_3OH product is taken from radiances measured by the radiometer centered near 640 GHz. However, as the methanol spectral signature in this region is very similar to that of ClO, additional measurements from the 190-GHz radiometer (which has channels sensitive to ClO but not CH_3OH) are used to decouple the CH_3OH and ClO information. CH_3OH was a new product in v4.2*x*; its quality has never been fully validated, and the scientific utility of the v5.0*x* MLS CH_3OH measurements remains to be determined. A summary of the estimated precision, resolution (vertical and horizontal), and systematic uncertainty of the v5.0*x* CH_3OH measurements as a function of altitude is given in Table 3.5.1.

3.5.2 Differences between v4.2*x* and v5.0*x*

CH_3OH abundances at 147 hPa have been reduced considerably in v5.0*x*, especially at low latitudes (Figure 3.5.1). This change likely represents a mild improvement, as preliminary comparisons with correlative measurements and model results had suggested that v4.2*x* CH_3OH mixing ratios were generally too high. However, although the substantial high bias at low latitudes at 147 hPa has been mitigated, many CH_3OH values at higher latitudes at that level that had been negative in v4.2*x* are now even more strongly negative, leading to a near-zero global-mean value there (as at other levels, not shown). Moreover, the overall systematic uncertainty in the data has increased in v5.0*x* (see Section 3.5.6).

3.5.3 Resolution

The resolution of the retrieved data can be described using "averaging kernels" [e.g., *Rodgers*, 2000]; the two-dimensional nature of the MLS data processing system means that the kernels describe both vertical and horizontal resolution. Values of the integrated kernel near unity indicate that the majority of information for that level has come from the measurements themselves and not the a priori; Figure 3.5.2 shows that the measurements dominate throughout most of the vertical range. Smoothing, imposed on the retrieval system in both the vertical and horizontal directions to enhance retrieval stability and precision, degrades the inherent resolution of the measurements. Thus, although CH_3OH measurements are reported at six pressure levels per decade change in pressure (spacing of ∼2.7 km), the vertical resolution of the v5.0*x* CH_3OH data as determined from the full width at half maximum of the rows of the averaging kernel matrix shown in Figure 3.5.2 is ∼3.5 km at 147 hPa and ∼5 km at 100 hPa. Figure 3.5.2 also shows horizontal averaging kernels, from which the along-track horizontal resolution is determined to be ∼150–350 km. The cross-track resolution, set by the width of the field of view of the 640-GHz radiometer, is ∼3 km. The along-track separation between adjacent retrieved profiles is 1.5° great circle angle (∼165 km), whereas the longitudinal separation of MLS measurements, set by the Aura orbit, is 10°–20° over low and middle latitudes, with much finer sampling in the polar regions.

3.5.4 Precision

The precision of the MLS CH_3OH data is estimated empirically by comparing profiles measured at the intersections of ascending (mainly day) and descending (mainly night) portions of the orbit. Under

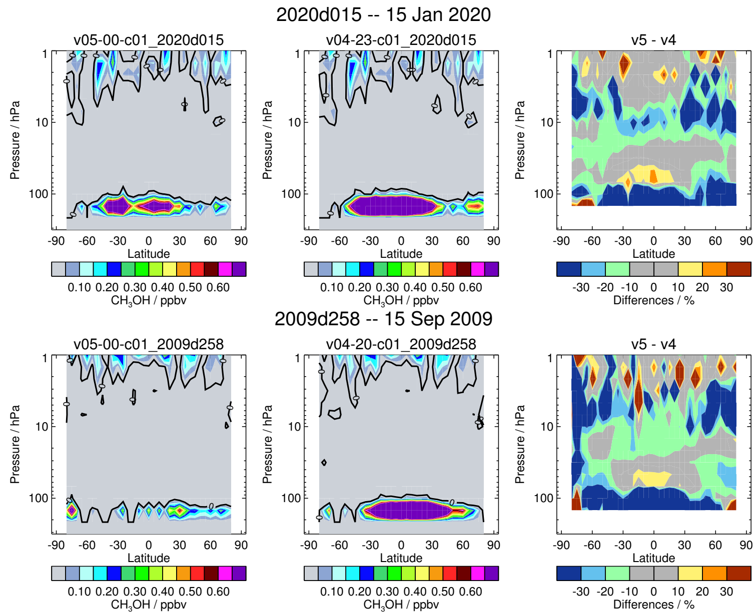

Figure 3.5.1: Zonal mean pressure-latitude cross sections of MLS CH_3OH, for (left) v5.0x, (middle) v4.2x, and (right) their differences (v5.0x minus v4.2x, in percent). Results are shown for two representative days in different seasons. The black curves overlaid on the abundance panels (left and middle) mark the zero contour.

ideal conditions (i.e., a quiescent atmosphere), the standard deviation about the mean differences between such matched profile pairs provides a measure of the precision of the individual data points. In practice, however, real changes in the atmosphere may occur over the 12 h interval between the intersecting measurement points, in which case the observed scatter provides an upper limit on the estimate of precision, assuming that the a priori has a negligible influence on the retrieval (a reasonable assumption throughout the retrieval range for CH_3OH). The precision estimates were found to be essentially invariant with time; results for several months of a representative year of data are shown in Figure 3.5.3. For the most part, differences between paired profiles are small, implying the absence of significant systematic ascending / descending biases. The observed standard deviation is $\sim$1 ppbv at 147 hPa. The observationally determined precision agrees well with that reported for each data point by the Level 2 data processing system. The estimates reported here represent the precisions at each pressure level of a single profile; precision can generally be improved by averaging, with the precision of an average of N profiles being $1/\sqrt{N}$ times the precision of an individual profile (although the actual standard error of the mean can in some cases be even smaller [*Toohey and von Clarmann*, 2013]).

3.5.5 Range

The MLS science team should be consulted before embarking on research using the CH_3OH product. CH_3OH is retrieved (and reported in the L2GP files) over the range 147 to 0.001 hPa. However, zonal mean mixing ratios are negative everywhere at retrieval pressures less than 100 hPa, as well as at middle and high latitudes at 100 hPa. Thus, with rare exceptions (such as during extreme events), the v5.0*x* CH_3OH data are considered potentially useful for scientific studies only at 147 hPa and at low latitudes at 100 hPa.

3.5.6 Accuracy

The effects of various sources of systematic uncertainty (e.g., instrumental issues, spectroscopic uncertainty, and approximations in the retrieval formulation and implementation) on the MLS v5.0*x* CH_3OH

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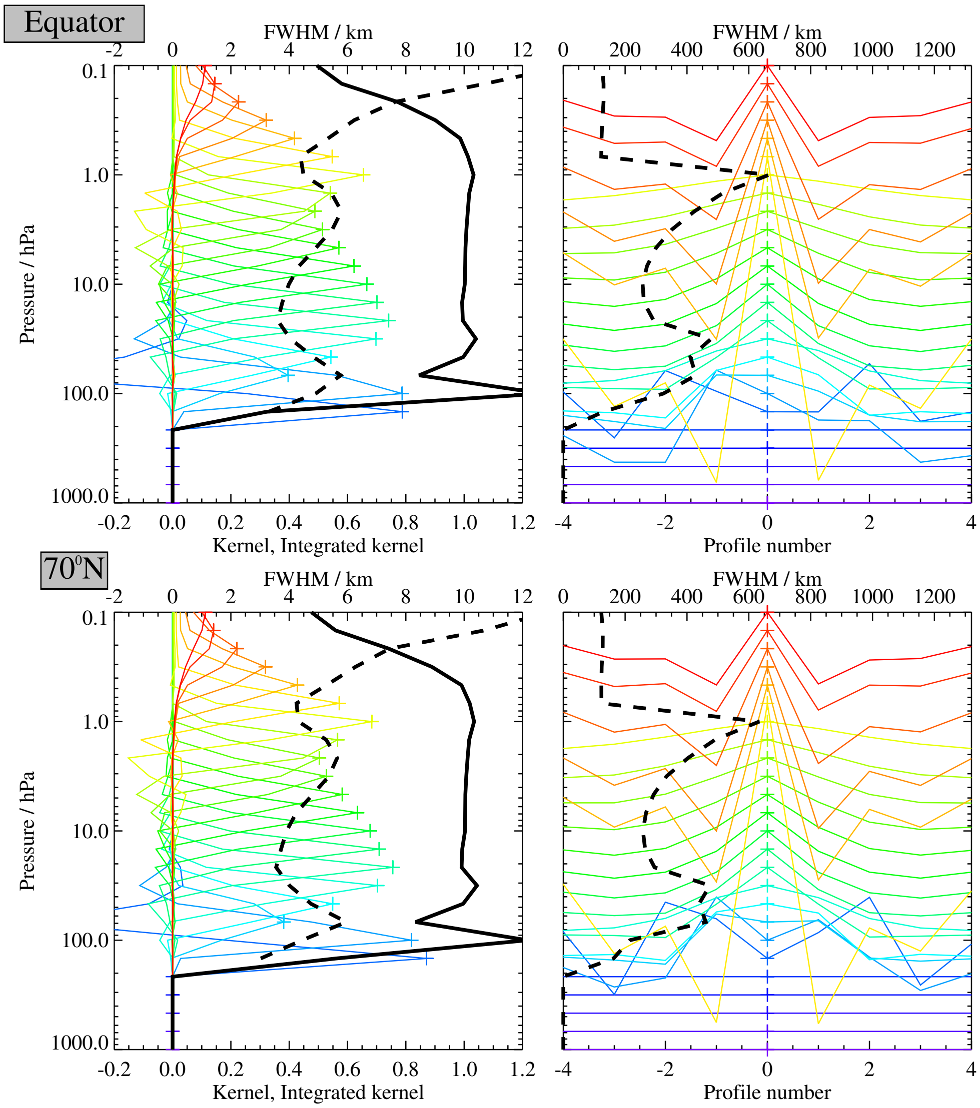

Figure 3.5.2: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x CH_3OH data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

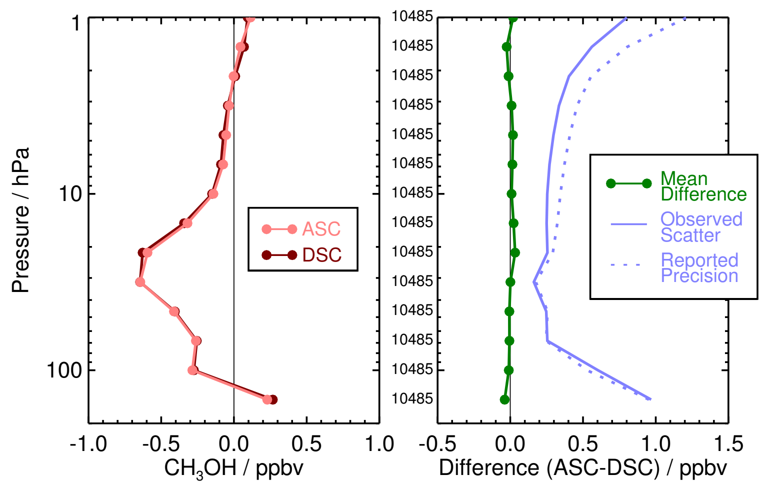

Figure 3.5.3: (left) Ensemble mean profiles for ascending (light red) and descending (dark red) orbit matching pairs of MLS v5.0x CH_3OH profiles averaged over several months of a representative year of data (2009). Symbols indicate MLS retrieval pressure levels. (right) Mean differences (ascending—descending) in pptv (green solid line). Also shown are the standard deviations about the mean differences (light blue solid line) and the root sum square (RSS) of the precisions calculated by the retrieval algorithm for the two sets of profiles (light blue dotted line). The observed scatter about the mean differences and the reported precision values have been scaled by $1/\sqrt{2}$ (to convert from standard deviations of differences into standard deviations of individual data points); hence the light blue solid line represents the statistical repeatability of the MLS measurements, and the light blue dotted line represents the expected 1σ precision for a single profile. The thin black lines mark zero in each panel. The number of crossing pairs of measurements being compared at each pressure level is noted in the space between the panels.

measurements have been quantified through a comprehensive set of retrievals of synthetic radiances. The overall systematic uncertainty, or accuracy, is calculated by combining (RSS) the contributions from both the expected biases and the additional scatter each source of uncertainty may introduce into the data. In aggregate, the factors considered in these simulations are estimated to give rise to total systematic uncertainty of approximately 150–400% in the MLS v5.0*x* CH_3OH data (see Table 3.5.1). These values for the overall uncertainty in v5.0*x* CH_3OH are slightly larger (poorer accuracy) than those estimated for the v4.2*x* data [see *Livesey et al.*, 2020].

3.5.7 Review of comparisons with other datasets

Detailed comparisons with correlative data sets have not been undertaken, but preliminary comparisons with version 3 ACE-FTS data suggested that the v4.2*x* MLS values may have been biased substantially high at 147 hPa (not shown). As noted above, CH_3OH abundances at 147 hPa have been reduced considerably in v5.0*x* and thus may be in better agreement with ACE-FTS data.

3.5.8 Data screening

Do not use: The v5.0*x* CH_3OH data should only be used in consultation with the MLS science team.

3.5.9 Artifacts

- A complete assessment of artifacts in the v5.0*x* CH_3OH measurements has not been performed, but it is known that zonal mean mixing ratios are negative everywhere at retrieval pressures less than or equal to 68 hPa, as well as at middle and high latitudes at 100 hPa.

3.5.10 Desired improvements for future data version(s)

- Specific achievable improvements in the CH_3OH retrieval remain to be determined.

Table 3.5.1: Summary of Aura MLS v5.0x CH_3OH Characteristics

Pressure / hPa	Resolution V × H[a] / km	Precision[b] / ppbv	Systematic Uncertainty[c] / %	Known Artifacts or Other Comments
68–0.001	—	—	—	Unsuitable for scientific use
100	5 × 350	±1	±150	Consult with MLS science team
147	3.5 × 150	±1	±400	Consult with MLS science team
1000–215	—	—	—	Not retrieved

[a] Vertical and Horizontal resolution in along-track direction.
[b] Precision on individual profiles.
[c] Values should be interpreted as 2-σ estimates of the probable magnitude.

3.6 Chlorine Monoxide (ClO)

Swath name: `ClO`

Useful range: 147–1.0 hPa

Contact: Michelle Santee, **Email:** <Michelle.L.Santee@jpl.nasa.gov>

3.6.1 Introduction

As in previous versions, in v5.0*x* the standard ClO product is derived from radiances measured by the radiometer centered near 640 GHz. ClO is also retrieved using radiances from the 190-GHz radiometer, but those data have poorer precision and larger biases and are not used in the standard ClO product. The quality and reliability of the version 2 (v2.2) Aura MLS ClO measurements were assessed in detail by *Santee et al.* [2008]. The ClO product was significantly improved in v3.3*x*/v3.4*x* [*Livesey et al.*, 2013]; in particular, the substantial (∼0.1–0.4 ppbv) negative bias present in the v2.2 ClO values at retrieval levels below (i.e., pressures larger than) 22 hPa was mitigated to a large extent, primarily through retrieval of CH_3Cl, which was a new MLS product in v3.3*x*/v3.4*x*. The ClO retrieval was largely unchanged over much of the profile in v4.2*x*, and the v5.0*x* retrieval does not depart dramatically from v4.2*x*, although the biases present at the lowest retrieval levels have been further reduced (see Section 3.6.5). The MLS v5.0*x* ClO data are scientifically useful over the range 147 to 1 hPa. A summary of the estimated precision, resolution (vertical and horizontal), and systematic uncertainty of the v5.0*x* ClO measurements as a function of altitude is given in Table 3.6.1.

3.6.2 Resolution

The resolution of the retrieved data can be described using "averaging kernels" [e.g., *Rodgers*, 2000]; the two-dimensional nature of the MLS data processing system means that the kernels describe both vertical and horizontal resolution. Smoothing, imposed on the retrieval system in both the vertical and horizontal directions to enhance retrieval stability and precision, degrades the inherent resolution of the measurements. Thus, although ClO measurements are reported at six pressure levels per decade change in pressure (spacing of ∼2.7 km), the vertical resolution of the v5.0*x* ClO data as determined from the full width at half maximum of the rows of the averaging kernel matrix shown in Figure 3.6.1 is ∼3–4.5 km throughout the retrieval range (with a mean of ∼3.5 km). The averaging kernels are sharply peaked at all levels, even at 147 hPa, where the kernel indicates that the retrieval has sensitivity to ClO abundances higher in the atmosphere (particularly 100 hPa). Nevertheless, the 147 hPa surface provides independent information. Figure 3.6.1 also shows horizontal averaging kernels, from which the along-track horizontal resolution is determined to be ∼300–500 km over most of the vertical range. The cross-track resolution, set by the width of the field of view of the 640-GHz radiometer, is ∼3 km. The along-track separation between adjacent retrieved profiles is 1.5° great circle angle (∼165 km), whereas the longitudinal separation of MLS measurements, set by the Aura orbit, is 10°–20° over low and middle latitudes, with much finer sampling in the polar regions.

3.6.3 Precision

The precision of the MLS ClO measurements is estimated empirically by computing the standard deviation of the descending (i.e., nighttime) profiles in the 20°-wide latitude band centered around the equator. For this region and time of day, natural atmospheric variability should be negligible relative to the measurement noise. As shown in Figure 3.6.2, the observed scatter in the data is virtually unchanged in v5.0*x*, ranging from ∼0.1 ppbv over the interval 100–3 hPa to ∼0.2 ppbv at 147 hPa and ∼0.3 ppbv at 1 hPa. The smoothing of the retrieval is turned off above 1 hPa, and as a consequence the

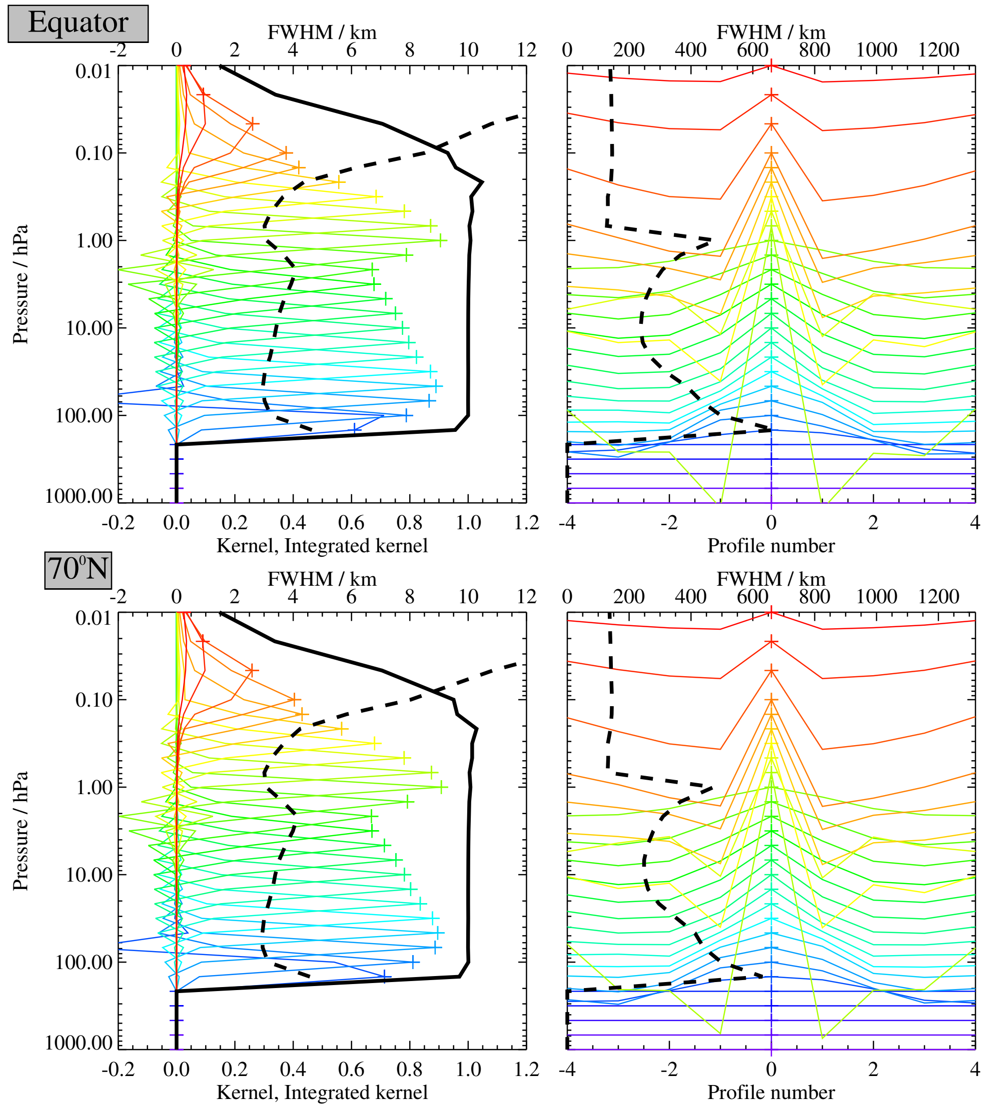

Figure 3.6.1: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x ClO data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

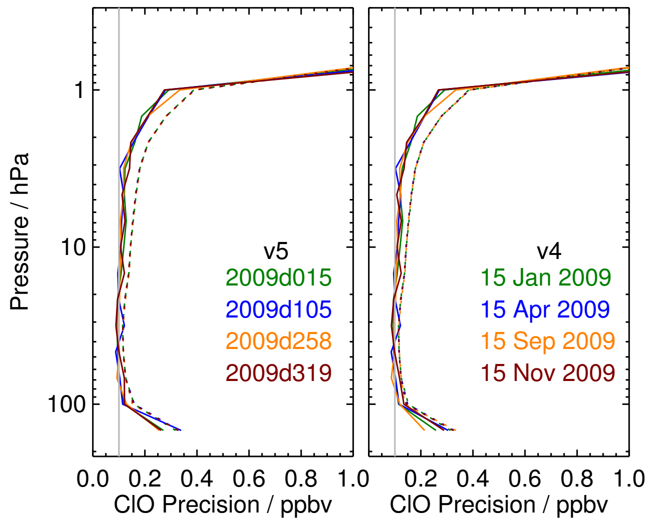

Figure 3.6.2: Precision of the (left) v5.0x and (right) v4.2x MLS ClO measurements for four representative days in different seasons (see legend). Solid lines depict the observed scatter in nighttime (descending) measurements obtained in a narrow equatorial band (see text); dotted lines depict the theoretical precision estimated by the retrieval algorithm. The light grey vertical line marks 0.1 ppbv, the estimated single-profile precision over most of the recommended vertical range in both versions.

precision worsens steeply above this level. The scatter in the data is essentially invariant with time, as seen by comparing the results for the different days shown in Figure 3.6.2.

The single-profile precision estimates cited here are, to first order, independent of latitude and season, but of course the scientific utility of individual MLS profiles (i.e., signal to noise) varies with ClO abundance. Outside of the lower stratospheric winter polar vortices, within which ClO is often strongly enhanced, the single-profile precision exceeds typical ClO mixing ratios, necessitating the use of averages for scientific studies. Precision can generally be improved by averaging, with the precision of an average of N profiles being $1/\sqrt{N}$ times the precision of an individual profile (although the actual standard error of the mean can in some cases be even smaller [*Toohey and von Clarmann*, 2013]).

The observational determination of the precision is compared in Figure 3.6.2 to the theoretical precision values reported by the Level 2 data processing algorithms. The predicted precision exceeds the observed scatter, particularly above 15 hPa, indicating that the vertical smoothing (regularization) applied to stabilize the retrieval and improve the precision has a non-negligible influence on the results at these levels. Because the theoretical precisions take into account occasional variations in instrument performance, the best estimate of the precision of an individual data point is the value quoted for that point in the L2GP files, but it should be borne in mind that this approach slightly overestimates the actual measurement noise.

3.6.4 Accuracy

The effects of various sources of systematic uncertainty (e.g., instrumental issues, spectroscopic uncertainty, and approximations in the retrieval formulation and implementation) on the MLS v5.0*x* ClO measurements have been quantified through a comprehensive set of retrievals of synthetic radiances; see *Santee et al.* [2008] for details of a similar analysis conducted on MLS v2.2 ClO data. The overall systematic uncertainty, or accuracy, is calculated by combining (RSS) the contributions from both the expected biases and the additional scatter each source of uncertainty may introduce into the data. In aggregate, the factors considered in these simulations are estimated to give rise to a total systematic uncertainty ranging from approximately 0.02 to 0.6 ppbv, depending on the level, in the MLS v5.0*x* ClO data (see Table 3.6.1). These values for the overall uncertainty in v5.0*x* ClO, which are slightly larger (poorer accuracy) at 100 and 147 hPa than those estimated for the v4.2*x* data [see *Livesey et al.*, 2020], do not take into account the known biases in MLS ClO data at the lowest retrieval levels discussed in the following subsection.

3.6.5 Quantification and correction of biases in v4.2*x* and v5.0*x*

As with other species retrieved from the MLS 640-GHz receiver, lower stratospheric signals for ClO are affected by water vapor. Therefore, for the retrieval phase CorePlusR4AB14, which includes ClO (see Table 2.3.1), water vapor is constrained to the values from the MLS H_2O standard product. As discussed in Section 3.9.2, the dry bias below the tropopause present in earlier MLS data versions has been mitigated in v5.0*x*. Some of the differences between v5.0*x* and v4.2*x* ClO can thus be attributed to the improvement in H_2O between the two versions. Zonal-mean differences from v4.2*x* are generally small (less than 10%) except at the bottom of the retrieval range (68–147 hPa), where low ClO abundances lead to larger percent differences (Figure 3.6.3). Figure 3.6.4 depicts v5.0*x* and v4.2*x* nighttime mixing ratios for a representative day during winter (when ClO is enhanced in the sunlit polar lower stratosphere) in both the Northern and Southern Hemispheres, and mean daytime and nighttime vertical profiles from the two versions are compared in the tropics and the Northern and Southern Hemisphere polar regions for the same two days in Figure 3.6.5; plots for other days give similar results (not shown). The two versions are in very close agreement at higher levels, including around the secondary peak in the ClO profile in the upper stratosphere (Figure 3.6.5). In addition to the standard product (derived from the 640-GHz radiances), Figure 3.6.5 includes results for the product retrieved from the 190-GHz radiances. The very large negative bias in `ClO-190` at its lowest retrieval levels (68–100 hPa) has been greatly reduced in v5.0*x*; thus the two ClO products correspond more closely now than they did in v4.2*x*. Nevertheless, both continue to display non-negligible biases that need to be corrected before being used in detailed quantitative studies (as was the case for previous versions of the MLS ClO data).

Figures 3.6.3–3.6.5 show that the differences between the two versions are larger at the lowest retrieval pressure levels, where substantial biases present in v4.2*x* have been ameliorated in v5.0*x*. To investigate in more detail the magnitude of and temporal variations in the bias in the v5.0*x* MLS ClO data and compare them to v4.2*x*, we show in Figure 3.6.6 monthly zonal means of MLS nighttime ClO measurements for pressure levels 147–46 hPa. Each panel represents a calendar month; nighttime data taken during that month over the period 2005–2020 have been binned and averaged in 5°-wide latitude bands between ±85°. Figure 3.6.7 is a similar plot but encompasses all of the MLS nighttime ClO data (i.e., the climatological annual mean over 2005–2020) for pressure levels 147–10 hPa. In both figures, bold colors represent v5.0*x* data, while corresponding pale colors represent v4.2*x* data. To guide the eye, the global-mean annual-mean bias calculated over the climatological period is indicated for each pressure level (horizontal solid lines in the respective bold and pale colors). Figures 3.6.4, 3.6.6, and 3.6.7 show that the magnitude, and at 100 and 147 hPa even the sign, of the bias varies with latitude as well as pressure. At 46 hPa, a negligible negative bias present in v4.2*x* is further reduced in v5.0*x*. At 68 hPa, the small negative bias in v4.2*x* is considerably lessened but is still evident in v5.0*x*. At 100 hPa, the substantial negative bias at higher latitudes (in both hemispheres) is much smaller, but a slight positive bias is now seen in the tropics. At the latter two levels, the magnitude of the global-mean bias decreased by about half between v4.2*x* and v5.0*x*. At 147 hPa, both the large negative bias in the polar regions and the large positive bias at low latitudes are much smaller, such that the strong latitude dependence at this level in v4.2*x* has been somewhat flattened in v5.0*x*. However, unlike at 68 and 100 hPa, the global mean bias has increased slightly at 147 hPa in v5.0*x*. In contrast to the strong altitude and latitude dependence of the ClO bias evident in these plots, Figure 3.6.6 reveals only slight month-to-month variability in most places.

In many cases the ClO bias can be essentially eliminated by subtracting daily gridded or zonal-

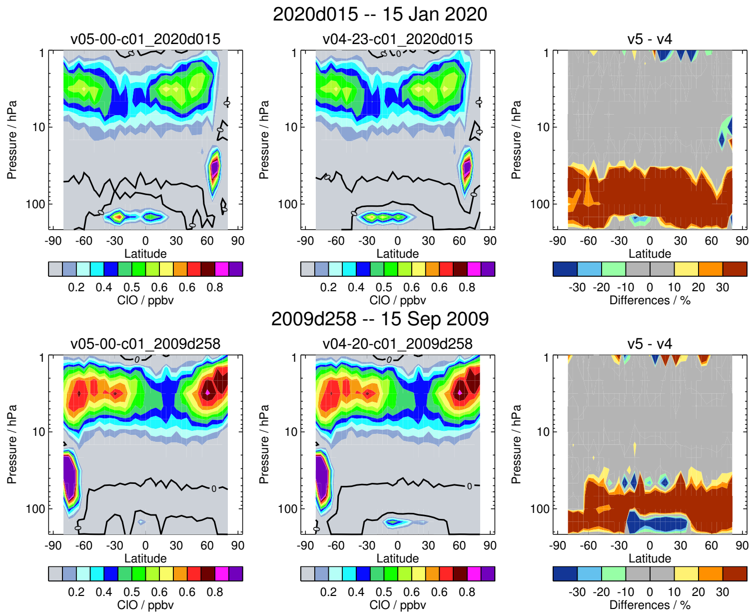

Figure 3.6.3: Zonal mean pressure-latitude cross sections of MLS daytime (ascending) ClO, for (left) v5.0x, (middle) v4.2x, and (right) their differences (v5.0x minus v4.2x, in percent). No bias corrections have been applied. Results from a representative day with strong ClO enhancement in the winter polar region are shown for (top panels) the Northern Hemisphere and (bottom panels) the Southern Hemisphere. The black curves overlaid on the abundance panels (left and middle) mark the zero contour.

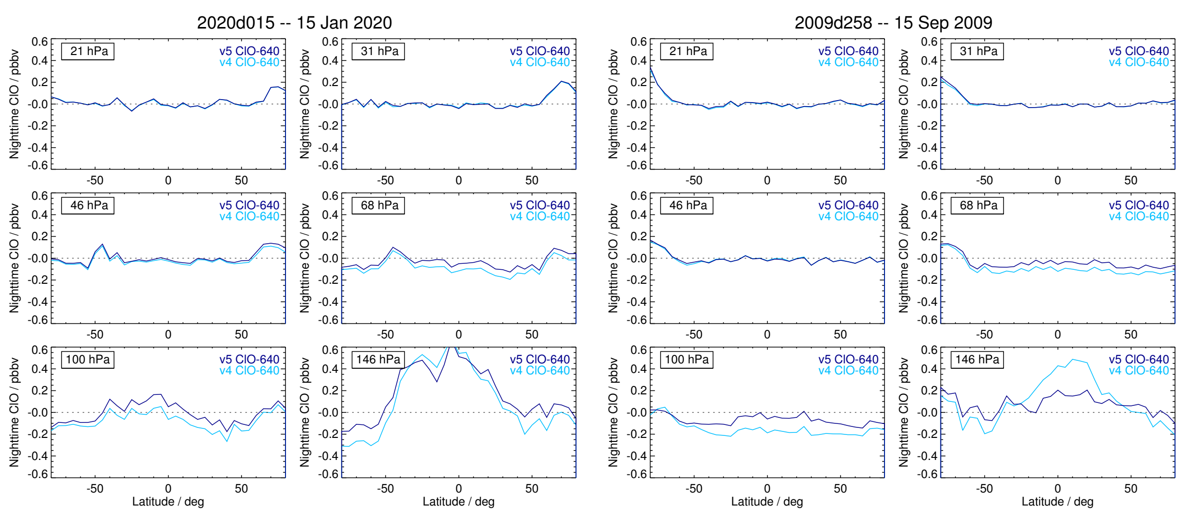

Figure 3.6.4: Nighttime v5.0x (dark blue) and v4.2x (light blue) MLS ClO data as a function of latitude for the six lowest retrieval pressure surfaces (21–147 hPa) for a representative day during winter in the Northern (left) and Southern (right) Hemispheres.

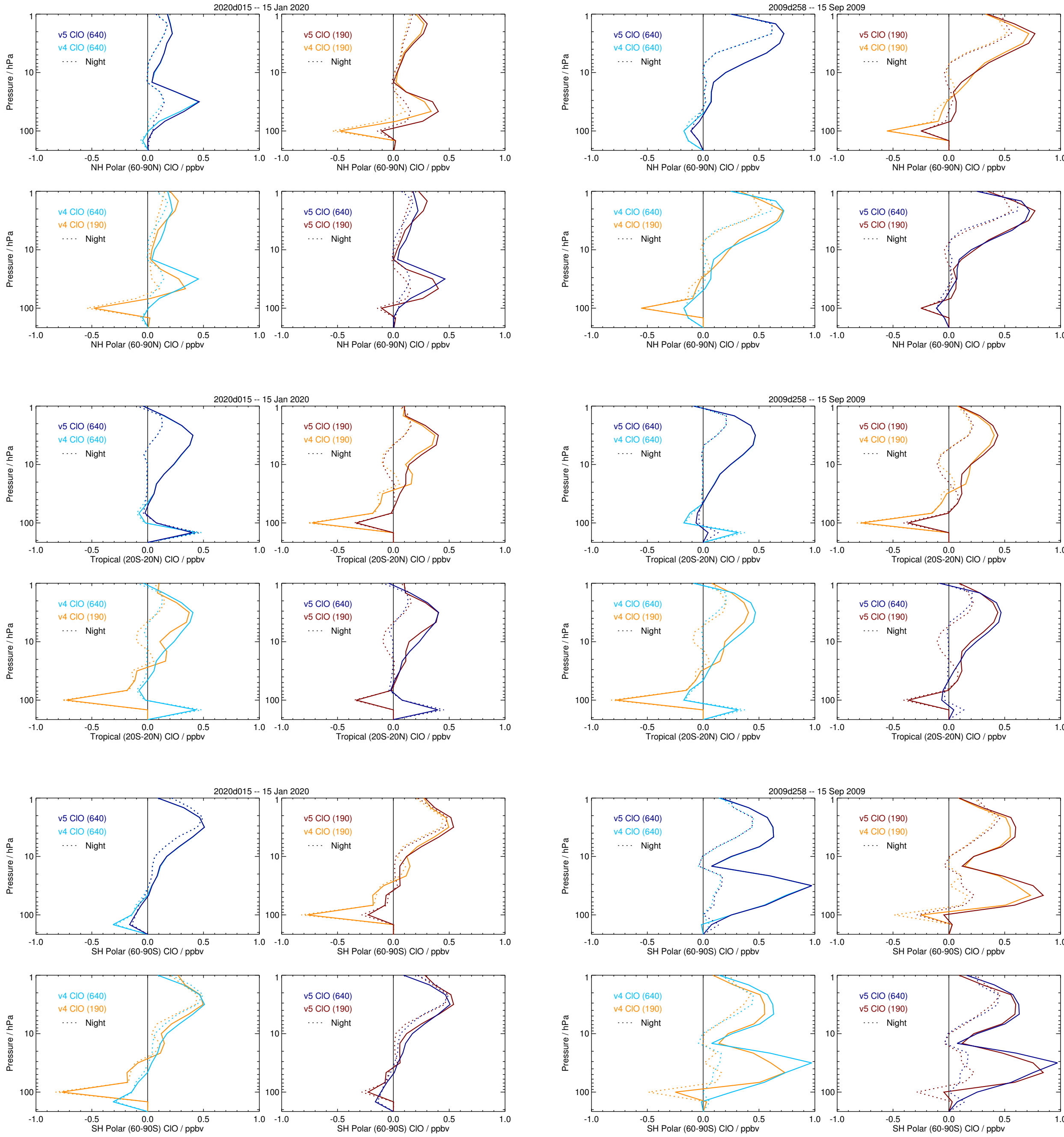

Figure 3.6.5: MLS v5.0x (dark colors) and v4.2x (light colors) profiles of `ClO-640` (blues) and `ClO-190` (reds) averaged over the Northern Hemisphere polar (top set), tropical (middle set), and Southern Hemisphere polar (bottom set) regions for a representative day during winter in the Northern (left side) and Southern (right side) Hemispheres. Each set of plots contains four panels, comparing v5.0x and v4.2x `ClO-640` retrievals, v5.0x and v4.2x `ClO-190` retrievals, v4.2x `ClO-640` and `ClO-190` retrievals, and v5.0x `ClO-640` and `ClO-190` retrievals. Solid lines show ascending (mainly daytime) and dashed lines show descending (mainly nighttime) averages.

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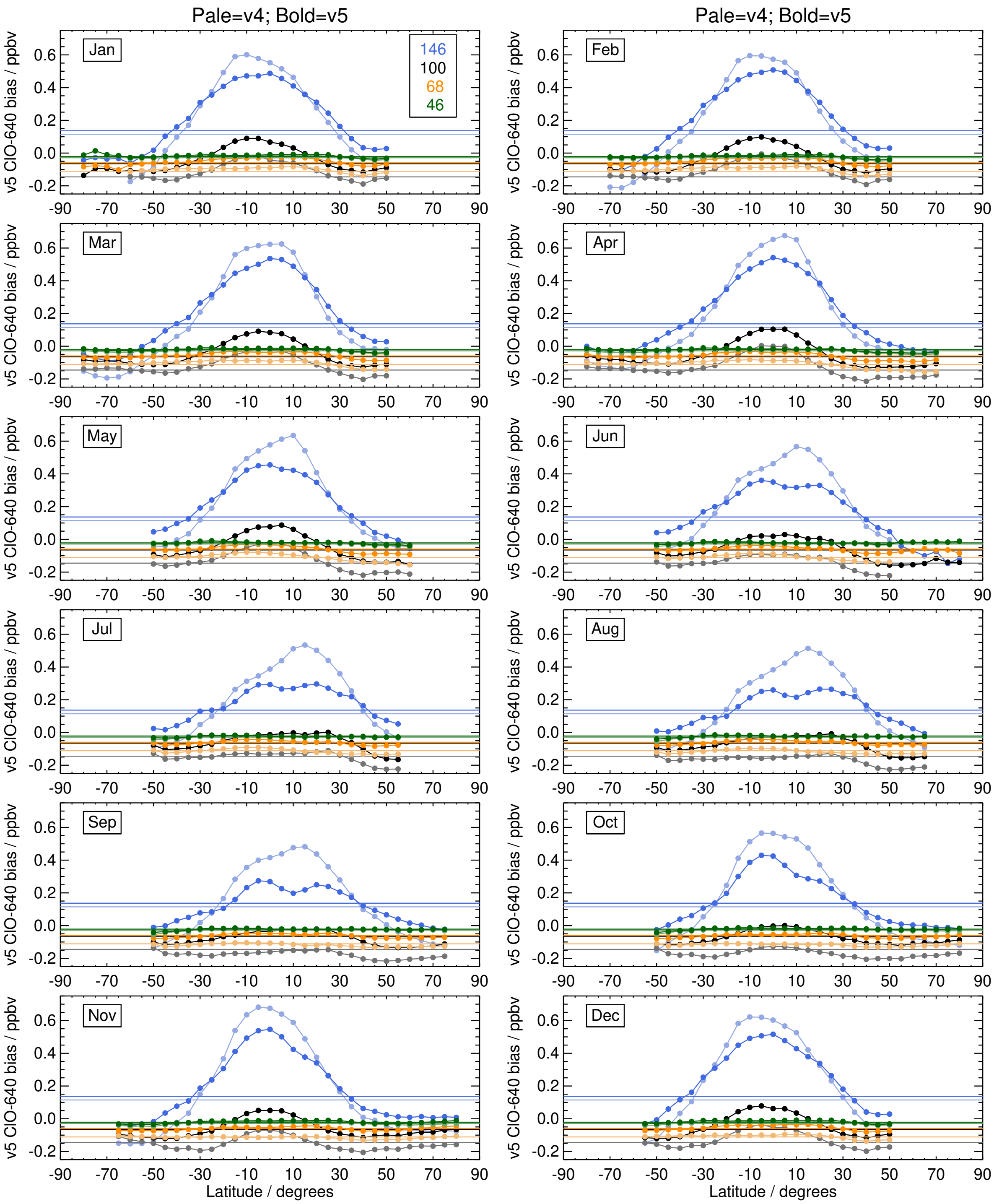

Figure 3.6.6: Estimates of the bias in MLS v5.0x ClO data in 5°-wide geographic latitude bands on the 147, 100, 68, and 46 hPa MLS retrieval pressure surfaces (see legend). Each panel shows monthly zonal means of v5.0x MLS nighttime (solar zenith angle > 100°) ClO measurements averaged over a 16-yr period (2005–2020, filled circles). Results for v5.0x are depicted in bold colors, those for v4.2x in corresponding pale colors. The horizontal lines denote the global-mean annual-mean bias estimates over the climatological period for both versions at each level. To ensure that ClO was not enhanced, consideration was restricted to latitudes equatorward of 50°S for the days between 1 May and 1 November and to latitudes equatorward of 50°N for the days between 1 December and 1 April.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

mean nighttime values from daytime measurements, and where feasible that is often the preferred bias-correction approach. However, it is not practical to do so under conditions of continuous daylight in the summer or continuous darkness in the winter at high latitudes. Moreover, under certain circumstances during the mid-winter period of peak ClO enhancement inside the lower stratospheric polar vortices, non-negligible ClO abundances can be present even in darkness, masking the negative bias. In this case, computing day—night differences considerably reduces the apparent degree of observed chlorine activation. Consequently, for studies of polar chemical processing and chlorine partitioning, it is instead recommended that an estimate of the bias be subtracted from the individual measurements at each affected retrieval level. Attempts to estimate the bias through approaches other than examination of nighttime ClO measurements (e.g., via correlations with potentially interfering species, which themselves may vary strongly with season) have so far met with little success. Thus the bias is estimated from the analysis depicted in Figure 3.6.7. Although monthly varying bias estimates might be desirable, as noted above seasonal variations are small, and it is not possible to directly quantify the bias in the polar regions during much of the year. Interannual variations and longer-term trends (not shown) in the magnitude of the bias are also small (especially in comparison to the uncertainty in the bias estimates and the v5.0*x* ClO data themselves; see Section 3.6.4). For these reasons, and to simplify application of the ClO bias correction for MLS data users, we report 16-yr climatological bias estimates that vary latitudinally and altitudinally but not temporally; these bias corrections should be adequate for most studies. The bias values, reported on a 5° grid, must be interpolated to the MLS Level 2 measurement locations being considered and subtracted from the ClO mixing ratios (daytime or nighttime) at those locations. The bias correction must be performed *before* interpolation to a different vertical coordinate (e.g., potential temperature). An ASCII file containing the estimated ClO bias values has been embedded in the PDF version of this document; instructions for extracting this file are given in Appendix A.2. The file is also available at `https://mls.jpl.nasa.gov/data/MLS-Aura_ClO-BiasCorrection_v05.txt`.

3.6.6 Review of comparisons with other data sets

Extensive comparisons of MLS v2.2 ClO data with measurements from a variety of different platforms (ground-based, balloon-borne, aircraft, and satellite) were presented by *Santee et al.* [2008]. A subset of those comparisons with v3.3*x*/v3.4*x* ClO data were reported by *Livesey et al.* [2013]. Comparisons of v5.0*x* ClO with correlative measurements have not been conducted but are expected to yield results similar to those for previous versions.

3.6.7 Data screening

Pressure range: 147–1.0 hPa

Values outside this range are not recommended for scientific use.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is zero.

We recommend that all profiles with nonzero values of `Status` be discarded, because of the potential impact of cloud artifacts at lower levels. Note, however, that rejecting in their entirety all profiles with nonzero `Status` may be unnecessarily severe at and above (i.e., at pressures equal to or smaller than) 46 hPa, where clouds have negligible impact; thus otherwise good-quality profiles with nonzero but even `Status` values may be used without restriction at those levels as long as they are removed at larger pressures. See Section 1.6 for more information on the interpretation of the `Status` field.

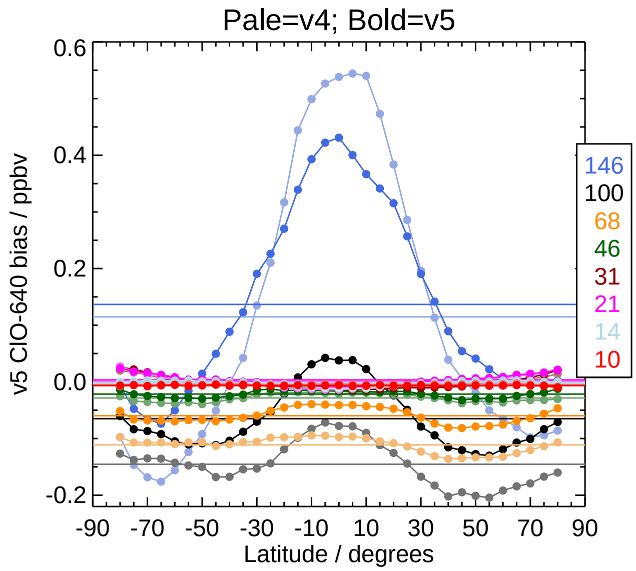

Figure 3.6.7: Estimates of the bias in MLS v5.0x nighttime (solar zenith angle > 100°) ClO data in 5°-wide geographic latitude bands on MLS retrieval pressure surfaces from 147 to 10 hPa (see legend) calculated over a 16-yr period (2005–2020). Results for v5.0x are depicted in bold colors, those for v4.2x in corresponding pale colors. The horizontal lines denote the global-mean annual-mean bias estimates over the climatological period for both versions at each level. To ensure that ClO was not enhanced, consideration was restricted to latitudes equatorward of 50°S for the days between 1 May and 1 November and to latitudes equatorward of 50°N for the days between 1 December and 1 April.

Quality: Only profiles whose `Quality` field is greater than 1.3 should be used.

This threshold for `Quality` (unchanged from v4.2*x*) typically excludes less than 0.5% of ClO profiles on a daily basis; note that it potentially discards some "good" data points while not necessarily identifying all "bad" ones.

Convergence: Only profiles whose `Convergence` field is less than 1.05 should be used.

On a typical day this threshold for `Convergence` (unchanged from v4.2*x*) discards very few (0.5% or less) of the ClO profiles, many (but not all) of which are filtered out by the other quality control measures.

3.6.8 Artifacts

- As discussed in Section 3.6.4, non-negligible biases are present in both daytime and nighttime v5.0*x* ClO mixing ratios at and below (i.e., pressures larger than) 68 hPa. The bias should be corrected by subtracting from the individual measurements at each affected retrieval level the altitude- and latitude-dependent bias estimates reported in an ASCII file that has been embedded in the PDF version of this document; instructions for extracting this file are given in Appendix A.2. This file is also available at `https://mls.jpl.nasa.gov/data/MLS-Aura_ClO-BiasCorrection_v05.txt`.
- Care must be taken in interpreting the ClO measurements immediately following severe pyrocumulonimbus (pyroCbs) events, which can rapidly loft polluted air from the surface and deposit it in the lower stratosphere. Air masses characterized by enhanced abundances of biomass burning pollutants may appear to also contain elevated levels of ClO, but such apparent enhancements

are artifacts induced by contamination of the ClO retrieval from methanol (CH_3OH), a product of wildfires that has a similar spectral signature in the MLS band used to measure ClO.

3.6.9 Desired improvements for future data version(s)

- Reduce the biases present at the lowest retrieval levels (147–68 hPa).

Table 3.6.1: Summary of Aura MLS v5.0x ClO Characteristics

Pressure / hPa	Resolution V × H[a] / km	Precision[b] / ppbv	Systematic Uncertainty[c] / ppbv	Known Artifacts or Other Comments
0.68–0.001	—	—	—	Unsuitable for scientific use
1.0	3 × 500	±0.3	±0.02	
6.8–1.5	3.5–4 × 250–350	±0.1	±0.02	
15–10	3.5 × 250	±0.1	±0.03	
22	3 × 300	±0.1	±0.05	
46–32	3 × 300–400	±0.1	±0.15	
68	3 × 450	±0.1	±0.2	Latitude-dependent bias[d]
100	3 × 500	±0.1	±0.3	Latitude-dependent bias[d]
147	4.5 × 650	±0.2	±0.6	Latitude-dependent bias[d]
1000–215	—	—	—	Not retrieved

[a] Vertical and Horizontal resolution in along-track direction.

[b] Precision on individual profiles, determined from observed scatter in nighttime (descending) data in a region of minimal atmospheric variability.

[c] Values should be interpreted as 2-σ estimates of the probable magnitude and, at the higher pressures, are the uncertainties after subtraction of the known bias.

[d] Correct for the bias by subtracting from the individual measurements at this level the latitude-dependent bias estimates (see Section 3.6.5).

3.7 Carbon monoxide (CO)

Swath name: `CO`

Useful range: 215–0.001 hPa

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Michael Schwartz (troposphere), **Email:** <Michael.J.Schwartz@jpl.nasa.gov>

3.7.1 Introduction

Carbon monoxide is retrieved from radiance measurements of two bands in the MLS 240 GHz radiometer. Full details are given in *Pumphrey et al.* [2007] and *Livesey et al.* [2008].

3.7.2 Differences between v5.0*x* and v4.2*x*

The v5.0*x* carbon monoxide (CO) product is generally similar to the v4.2*x* product in the upper troposphere and stratosphere, and has been improved in some cases in the mesosphere and mesopause region through the use of a more computationally expensive, nonlinear forward model for radiances near the 230-GHz line center. In the upper mesosphere, v5.0*x* CO is less tightly constrained to its *a priori* (*a priori* precision is 1.5× larger at 0.046 hPa and 2× larger at and above 0.01 hPa). Horizontal smoothing of v5.0*x* has been tightened at and above 0.01 hPa to maintain retrieval stability, but his change has no appreciable impact on the sharpness of horizontal features seen in preliminary validation. The vertical range of the retrieval has been extended to 0.00046 hPa and profiles are recommended for scientific use up to 0.001 hPa.

Improvement is most evident in cases where there are sharp vertical features, as are sometimes found in descending high values of CO in polar winter vortices. Figure 3.7.2 shows scatter plots between v5.0*x* and v4.2*x* CO for levels between 215 hPa and 0.01 hPa for 2009 data. Note that these histograms' colors are on a log scale, with the red colors along the 1:1 line several orders of magnitude more frequent than the blue colors. The highest values at levels between 0.464 hPa and 0.0215 hPa are in the reforming upper-level, northern-winter polar vortex after a sudden stratospheric warming; v5.0*x* better represents these descending high values while the highest values of v4.2*x* CO are pulled down toward *a priori*. Descending CO in the southern winter polar vortex reaching the middle stratosphere is also better represented in v5.0*x* between 31.6 hPa and 4.64 hPa; v4.2*x* profiles tended to be more oscillatory and more often included negative mixing ratios.

High outlier values of CO along the 1:1 lines of panels for 216–46.4 hPa in Figure 3.7.2 are from the plume of the "Black Saturday" Australian wildfires and confirm the consistency of the v5.0*x* and v4.2*x* retrievals in the upper troposphere and lower stratosphere.

3.7.3 Resolution

Figure 3.7.1 shows the horizontal and vertical averaging kernels for v5.0*x* MLS CO. Estimated vertical and horizontal resolutions are essentially very similar to those of v4.2*x*, with only slight improvement in the mesosphere, but the improved forward model allows the retrieval to provide a better representation of the atmosphere in the mesosphere. The vertical resolution is in the range 3.5–5 km from the upper troposphere to the lower mesosphere, degrading to 6–7 km in the upper mesosphere. Down to the 215 hPa level, the vertical averaging kernels are sharply peaked at the level being retrieved, but while the 316-hPa measurement contains contribution from 316 hPa, it has a larger contribution from 215 hPa and a negative contribution around 100 hPa of similar magnitude to that at 316 hPa. The retrieved value at 316 hPa is thus more an extrapolation of the profile higher in the UTLS than it is an independent measurement at 316 hPa, and it is not recommended for scientific use. The horizontal resolution is about 200 km in the mesosphere, degrading slowly to 300 km with decreasing height in the stratosphere and more rapidly to about 460 km at 100 hPa and 690 km at 215 hPa.

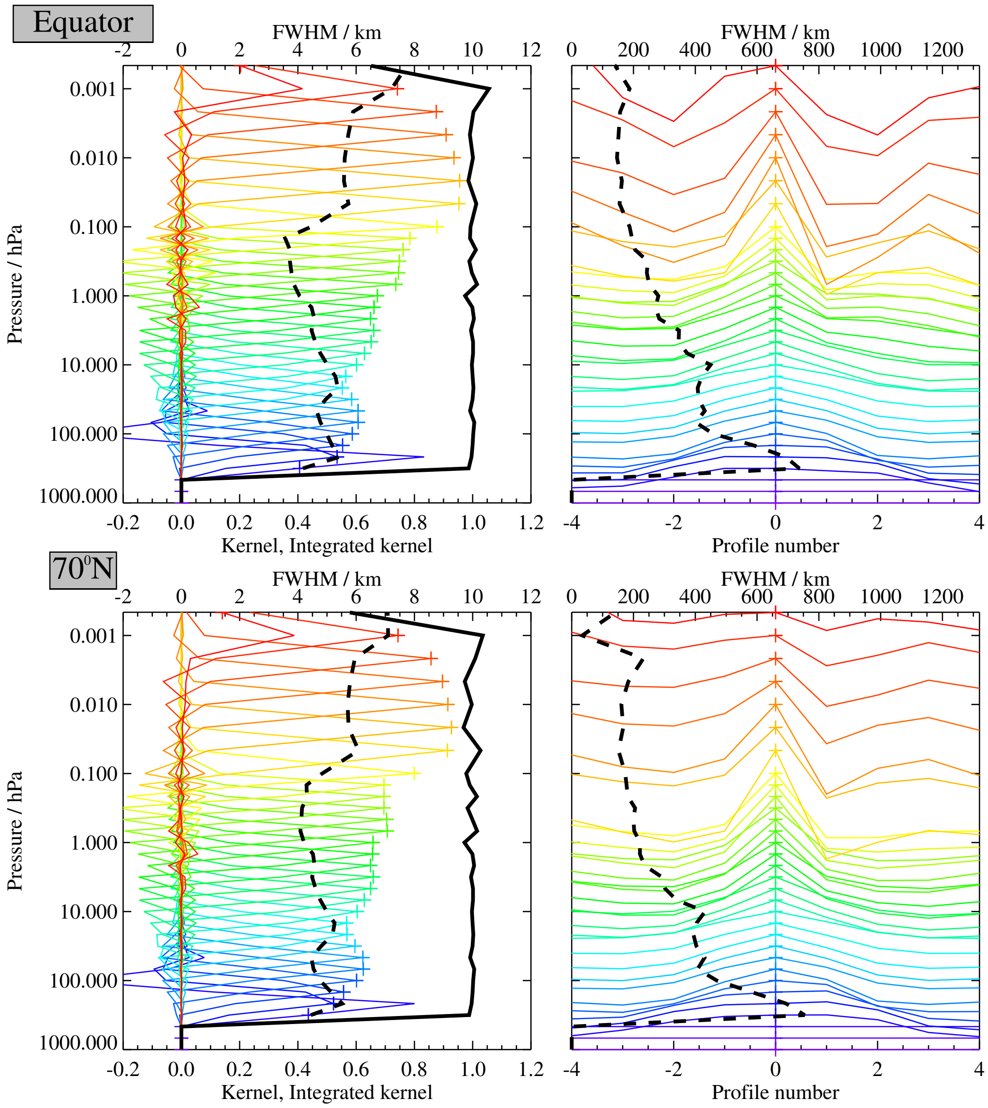

Figure 3.7.1: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x CO data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

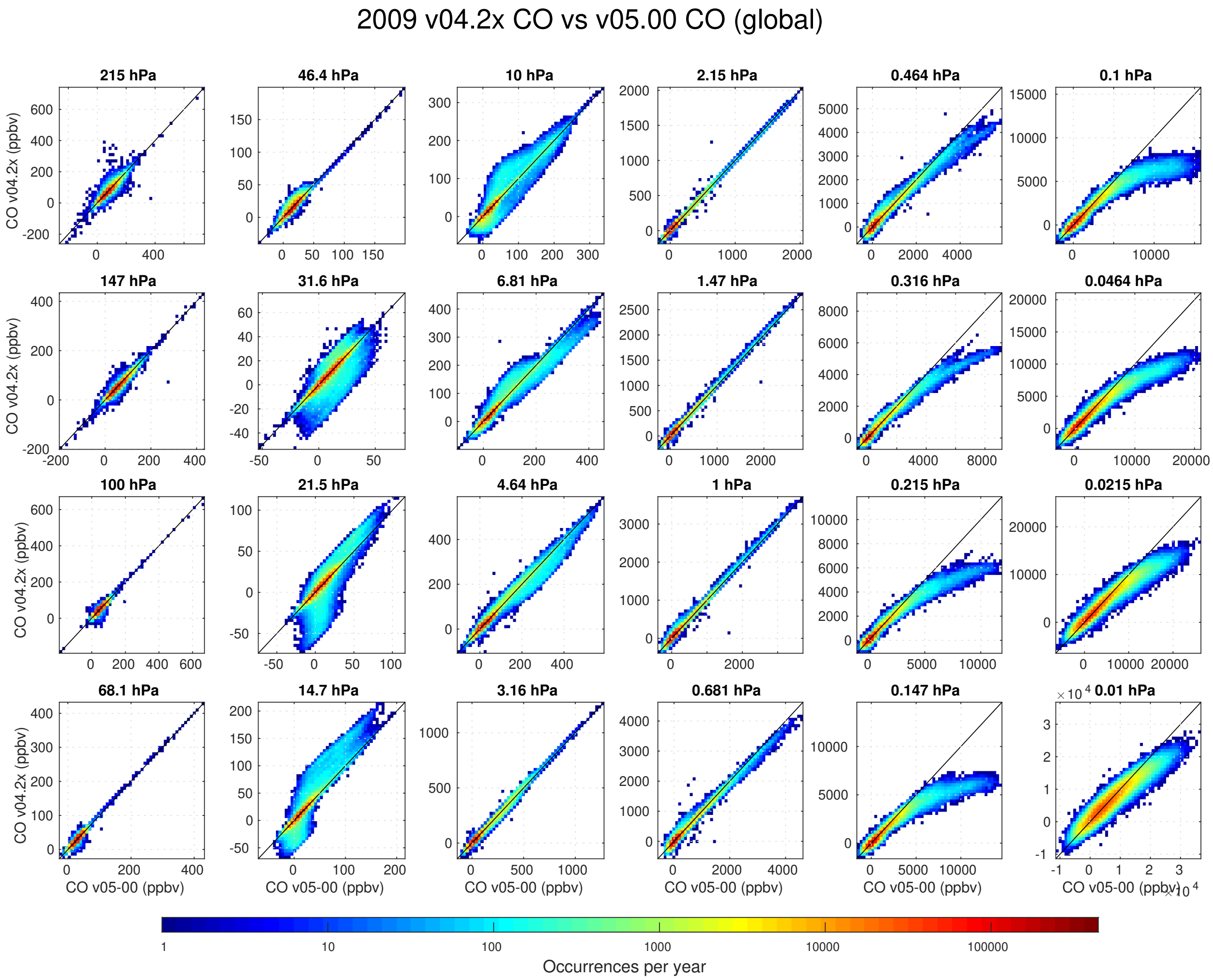

Figure 3.7.2: Joint histograms of v4.2x CO and v5.0x CO for 2009 data show the general consistency of the two versions as well as their departures. The color scale is logarithmic, with red points along the 1:1 line corresponding to pairs of values in good agreement between the versions, generally several orders of magnitude more common than v5.0x-v4.2x pairs that significantly disagree.

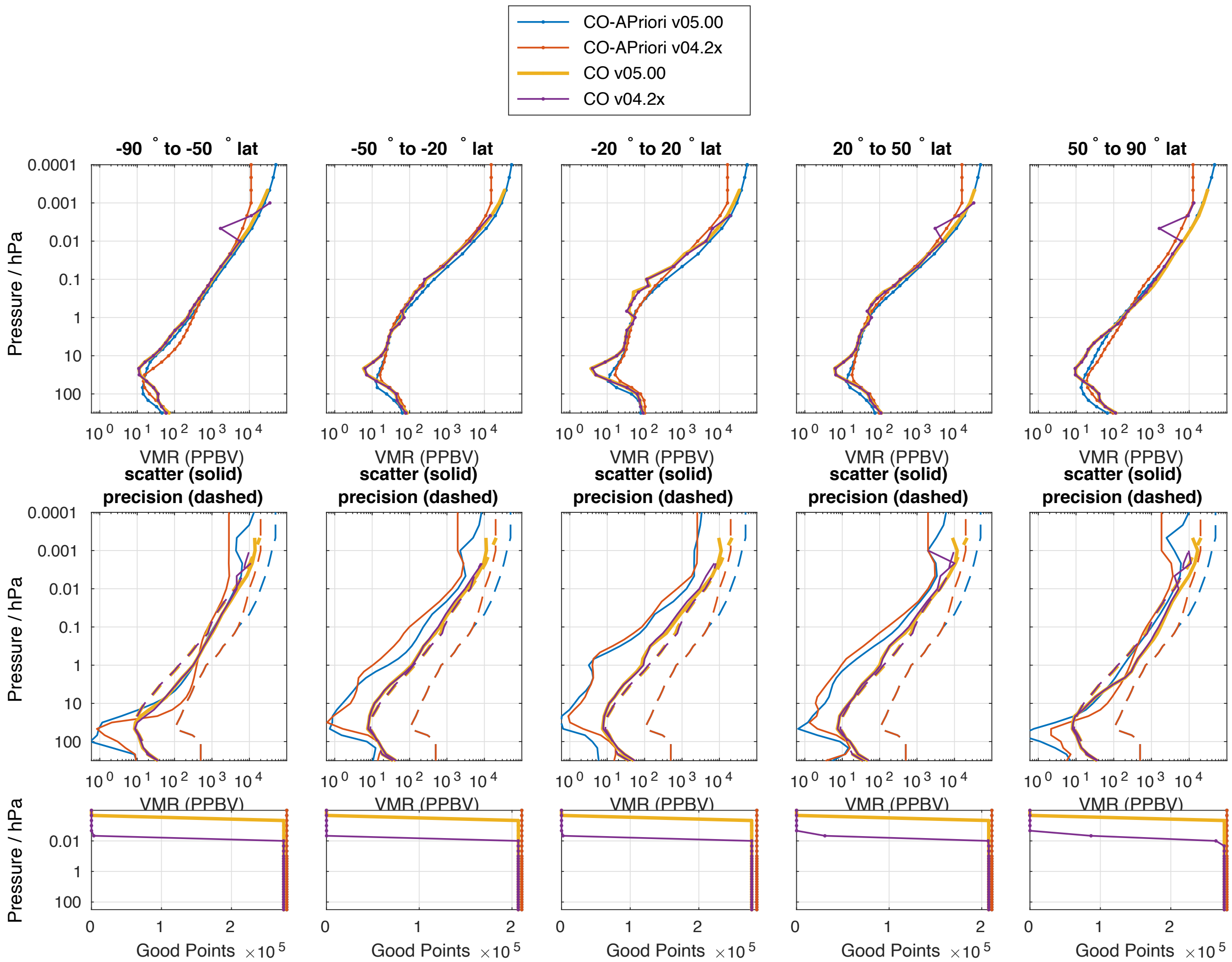

Figure 3.7.3: The top row shows 2009 zonal means of v5.0x and v4.2x mixing ratios and their a priori values. The v4.2x retrieved mixing ratio line (purple) lies on top of the v5.0x mixing ratio line (yellow) for all but the highest altitude pressure surfaces, despite significant differences in their a priori profiles. The middle row shows the zonal scatter about these zonal means (solid lines) and corresponding estimated precisions (dashed lines). The bottom row shows the number of good profiles, limited at the highest retrieval levels where retrieved precision exceeds half of the a priori precision.

3.7.4 Precision

The MLS data are supplied with an estimated precision (the field `L2gpPrecision`) which is the *a posteriori* precision as returned by the optimal estimation. The precision of the v5.0*x* CO is very similar to that of v4.2*x*. In both versions, the precision is greater than the scatter observed in the data in regions of low natural variability. This can be seen in the middle (low-latitude) panels of the second row of Figure 3.7.3, where the purple and yellow solid lines (scatter about the zonal means) have smaller values than the purple and yellow dashed lines (precisions). Where the estimated precision is greater than 50% of the *a priori* precision the data will be influenced by the *a priori* to an undesirably large extent. In such cases, `L2gpPrecision` is set to be negative (or zero in some cases) to indicate that the data should not be used. The v5.0*x* *a priori* precision has been relaxed above 0.1 hPa (blue dashed line departing from red dashed line in center panels of Figure 3.7.3), and the level at which the retrieved precision is more than half of this *a priori* precision typically moves up from 0.0046 hPa to 0.00046 hPa.

Note that the random errors (precisions) are larger than 100% of the mixing ratio for much of the

Help Overview Table BrO CH$_3$Cl CH$_3$CN CH$_3$OH ClO CO GPH H$_2$O HCl HCN HNO$_3$ HO$_2$ HOCl IWC IWP N$_2$O O$_3$ OH RHI SO$_2$ T Lvl 3

vertical range, meaning that significant averaging (e.g., daily zonal mean or weekly map) is typially needed to make use of the data.

3.7.5 Accuracy

The estimated accuracy is summarized in Table 3.7.1. In the middle atmosphere the accuracies are estimated by comparisons with the ACE-FTS instrument; see *Pumphrey et al.* [2007] for further details. The MLS v2.2 CO data at 215 hPa showed high (factor of ∼2) biases compared to other observations. The morphology, however, was generally realistic [*Livesey et al.*, 2008]. In v5.0*x* (as in v4.2*x*) this bias has been essentially eliminated through a change in the approach to modeling the background radiance upon which the CO spectral line sits, and a small reduction in the number of MLS spectral channels considered in the retrieval. Tropospheric (215–100 hPa) accuracies in Table 3.7.1 are 2-σ estimates obtained by propagating parameter uncertainties through a model of the measurement system, and are unchanged from those calculated for v4.2*x*.

3.7.6 Data screening

Pressure range: 215–0.001 hPa.

Values outside this range are not recommended for scientific use. Data at 0.00046 hPa represents a total column at and above that pressure level. Scientific use of these 0.00046 hPa data may be possible, but requires consultation with the MLS team.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Clouds: Clouds have no impact for pressures of 31 hPa or less. v5.0*x* and v4.2*x* are much less susceptible to cloud-induced artifacts than was v03.x, so screening of the CO product is considerably simplified compared to that recommended for v03.x, needing only application of the standard `Quality` and `Convergence` rules as described below. The low-cloud status bit, which was almost never set in v4.2*x* (0.002% of profiles), is set for 0.6% of profiles in v5.0*x*, but preliminary validation does not find this flag to be useful for data screening.

Quality: Only use profiles with `Quality` greater than 1.5.

Profiles with `Quality` less than or equal to 1.5 comprise 0.7% of all data, and ∼2% of profiles in the tropics. At 215 hPa in the tropics, the rejected profiles have mixing ratios that are, on average, 7% higher than other tropical values and the occurrence rates of high outliers with mixing ratios greater than 150 ppbv is about twice that of the rest of the tropical ensemble. At 100 hPa there is no significant difference in the means of tropical profiles with Quality less than or greater than 1.5.

Convergence: Only profiles whose `Convergence` field is less than 1.03 should be used.

This `Convergence` criterion rejects fewer than 0.1% of profiles. Almost all of the retrievals in the phase that produces v5.0*x* CO converge to their target, so `Convergence` is of limited use in screening.

3.7.7 Artifacts

- Positive systematic error of 20–50% throughout the mesosphere, as was the case for v4.2*x*.

- Negative systematic error of 50–70% near 30 hPa, as was the case for v4.2*x*.
- Retrieved profiles are rather jagged, especially between 1 hPa (48 km) and 0.1 hPa (64 km). The greater smoothing applied in v5.0*x*, v4.2*x* and v03.3 compared to v2.2 has reduced this problem considerably but has not eliminated it entirely.
- The tendency for negative values to occur at the level below a large positive value that was present in v4.2*x* is somewhat reduced in v5.0*x*.
- Upper-tropospheric v5.0*x* CO retrieved values still show some anomalous sensitivity to thick clouds associated with deep convection. The screening procedure based upon `Quality` and `Convergence` that is described above is generally effective in removing these artifacts.
- Negative outliers in UT CO have been observed in volcanic plumes, such as that from the eruption of Sarychev in June of 2009. These are likely the result of interference from spectral lines of a gas-phase plume component, and are a subject for further analysis and validation.

3.7.8 Review of comparisons with other datasets

In the upper troposphere, comparisons with various in situ CO observations (NASA DC-8, WB-57 and the MOZAIC dataset) indicate that the *earlier* MLS v2.2 215 hPa CO product was biased high by a factor of ∼2. As in v4.2*x*, this bias is largely eliminated in v5.0*x*.

In the mesosphere, comparisons of the earlier v2.2 MLS CO with ODIN-SMR and ACE-FTS suggest a positive bias: 30%–50% against ACE-FTS, 50%–100% against SMR. Near 31 hPa, the MLS values are lower than SMR and ACE-FTS by at least 70%. The MLS values have not changed much between v2.2 and v5.0*x* in the middle atmosphere, so these comparisons may mostly be considered valid for v5.0*x*. What change there was between v2.2 and later versions consists of a slight lowering of the MLS values, bringing them slightly towards the ACE-FTS data; 20% is now a better estimate of the MLS-ACE bias in much of the middle atmosphere (compared to 30% with v2.2). Further validation of the v5.0*x* retrieval above 0.01 hPa is needed.

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

Table 3.7.1: Data quality summary for MLS v5.0x CO.

Pressure / hPa	Resolution / km Vert × Horiz.	Precision / ppbv	Accuracy	Comment
< 0.001	—	—	—	Not retrieved
0.00046	—	—	—	Unsuitable for scientific use
0.001	7.2 × 200	12000	validation needed	possibly use, with caution
0.0022	5.9 × 200	8700	validation needed	possibly use, with caution
0.0046	5.8 × 200	6000	+20% to +50%	
0.01	5.9 × 200	3400	+20% to +50%	
0.046	5.9 × 200	1000	+20% to +50%	
0.14	3.8 × 200	640	+20% to +50%	
1	4.1 × 250	120	+20% to +50%	
10	5.0 × 440	16	±10%	
31	4.9 × 400	9	−70% to −50%	
100	4.9 × 450	14	±19 ppbv and ±30% [a]	
147	5.1 × 570	16	±26 ppbv and ±30%	
215	5.4 × 690	19	±38 ppbv and ±30%	
316	—	—	—	Unsuitable for scientific use
>316	—	—	—	Not retrieved

[a] Estimated 215–100 hPa systematic uncertainty is the RSS of the additive and multiplicative terms.

3.8 Geopotential Height (GPH)

Swath name: GPH

Useful range: 261–0.00046 hPa

Contact: Michael J. Schwartz, **Email:** <Michael.J.Schwartz@jpl.nasa.gov>

3.8.1 Introduction

Geopotential height (GPH) is retrieved, along with temperature and the related assignment of tangent pressures to limb views, primarily from bands near O_2 spectral lines at 118 GHz and 234 GHz. The v5.0*x* GPH product is generally similar to the GPH products of earlier versions including the v02.2 product that is described in *Schwartz et al.* [2008] except that each profile is offset vertically in v5.0*x* so that its value at 100 hPa matches that of the GEOS-5.12.4 "Forward Processing for Instrument Teams" (FP-IT) GPH. In v4.2*x* and earlier versions, the absolute reference for GPH was inferred from the spacecraft orbit/attitude system and the instrument scan model. Throughout the rest of this section, "GEOS-5" without additional qualification refers to GEOS-5.12.4 FP-IT.

The heights of surfaces of constant geopotential are a property of the Earth's gravitational field and do not depend upon atmospheric conditions. Geopotential differences between surfaces are equal to the integral with height of the gravitational acceleration, g. GPH is geopotential difference from the Earth's surface geopotential to a given location, scaled by the mean-sea-level gravitational acceleration, g_0, to give units of height.

MLS products, including GPH and temperature, are reported on pressure surfaces, but pressure, temperature and height depend upon one another through assumed hydrostatic balance and the gas law.

$$\frac{1}{g_o}\int g\,dh = \frac{R}{M g_o}\int T\,dP/P, \tag{3.1}$$

where M is the molar mass of air and R is the gas constant. If we assume that we know the molar-mass profile of the atmosphere (which begins to vary significantly from its dry-air surface value in the mesosphere due to height-dependent changes in the mixing ratios of O_2 and N_2), then the retrieval of a temperature profile on fixed pressure surfaces also determines GPH differences between those surfaces, and so determines the GPH profile to within an additive constant. Absolute pointing cannot be inferred from radiometric information and must be obtained from *a priori* information, which was the spacecraft orbit/attitude system and instrument scan model in v4.2*x* and earlier versions and is GEOS 100 hPa GPH in v5.0*x*.

Table 3.8.1 summarizes v5.0*x* measurement precision, modeled accuracy and observed biases. The following sections provide details.

3.8.2 Differences between v5.0*x* and previous versions

The v5.0*x* and v4.2*x* GPH products are taken from the `CorePlusR3` retrieval phase (along with a number of standard products that depend upon radiances from the 240-GHz radiometer). The v02.2x and v03.x GPH products were taken from a preliminary retrieval phase.

The Earth Gravitational Model 1996 (EGM96) geoid defines zero height for GEOS-5 GPH, v5.0*x* GPH (which inherits this definition from GEOS-5), and v4.2*x* GPH. Earlier versions of MLS GPH used the WGS84 ellipsoid that is used in the MLS forward model ray tracing. The impact of this difference is discussed in the v4.2*x* version of this document.

The fill value for missing GPH data has been changed in v5.0*x* to -1×10^{15} m. The value of -999.99 m used for missing GPH data in v4.2*x* and earlier versions of MLS GPH is within the range

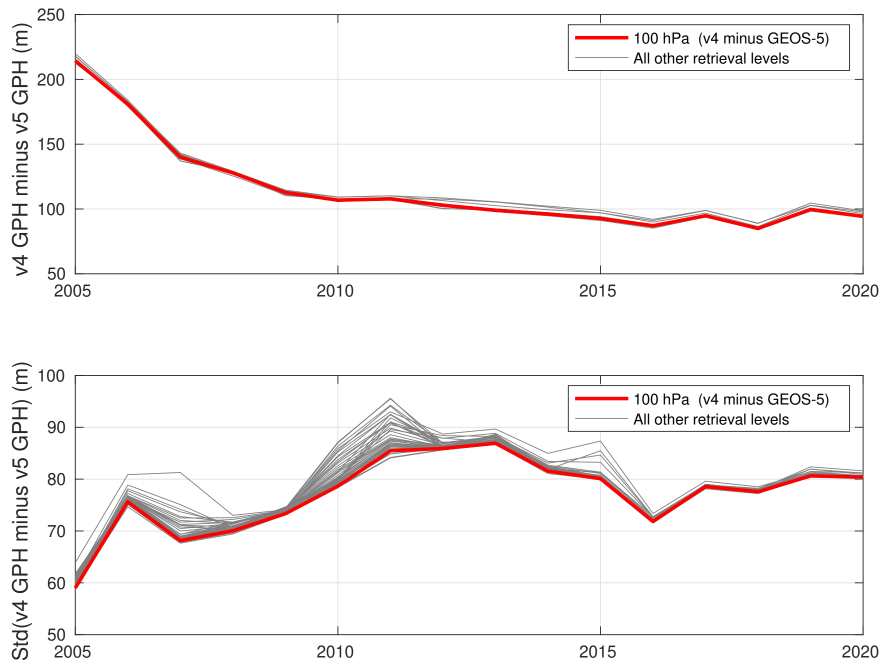

Figure 3.8.1: The top panel shows the daily mean difference between v5.0x and v4.2x GPH for January 15 of each year of MLS measurements to date. The red line highlights the differences at 100 hPa surface, for which the v5.0x values are GEOS-5, by construction, so is the trend of v4.2x minus GEOS-5. The gray lines are the daily-mean differences for all of the other retrieval levels, and show that these differences are dominated by the change at the reference level, with negligible contribution from the differences in integrated temperature of the two versions. The lower panel is the daily scatter in these differences, and shows that most of the scatter at all levels comes from the vertical offsets imposed by changing the 100 hPa level.

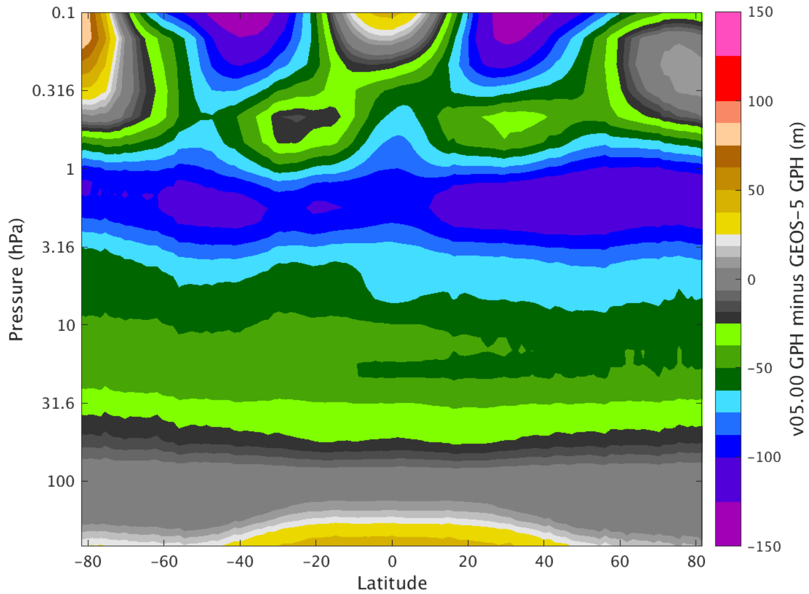

Figure 3.8.2: The zonal mean difference between GEOS-5 FP-IT GPH and MLS v5.0x GPH for the first 969 days processed with the v5.0x algorithms. This difference in GPH is zero, by construction, at 100 hPa, and away from the 100 hPa surface is the integral of the temperature biases between v5.0x and GEOS-5. Large differences in the mesosphere result from the GEOS-5 systems's lack of satellite temperature data for assimilation at these levels.

of valid GPH values that might be found at the bottom of a retrieval. Note that, while all v5.0*x* GPH files use the new -1×10^{15} m fill value, metadata for the v5.00 files incorrectly still quote −999.99 m as being the fill value; this is fixed in v5.01). In v5.01, the fill value for missing geolocation data remains −999.99, consistent with that used for other products (v5.00 inappropriately set these to -1×10^{15} m also).

3.8.3 Comparison to GEOS-5 Analysis

The v5.0*x* GPH product is identical to GEOS-5 at 100 hPa and differs at other levels to the extent that integrated temperature profiles of the two products differ. Mean differences shown in Figure 3.8.2, are less than 50 m magnitude in the upper troposphere and lower stratosphere. MLS GPH is 100 m lower than GEOS-5 FP-IT near the stratopause, and biases in the mesosphere are likely due to the lack of constraint of GEOS-5 temperature by assimilation at these levels.

A latitudinally and seasonally-varying bias between MLS v4.2*x* GPH and GEOS-5 GPH, shown in Figure 3.8.3, was the subject of extensive discussion in the v4.2*x* data quality document. Some of this annually-repeating "bias" may result from annually-repeating geophysical information captured by MLS that is not in the GEOS-5 analysis. However, the large ascending-descending differences are almost certainly not primarily diurnal effects. The fidelity with which these patterns annually repeat suggests that they may result from thermal distortions of the spacecraft/instrument that vary annually due to the eccentricity of the Earth's orbit, or from orbit/attitude errors from the star trackers that provide the spacecraft-attitude information. The same star fields are viewed each year at the same date and orbit position.

Elimination of this bias was a primary motivation for adopting GEOS-5 100 hPa GPH as an absolute reference height. Operational products from the GEOS-5 version that we are using for v5.0*x* processing,

Help Overview Table BrO CH$_3$Cl CH$_3$CN CH$_3$OH ClO CO GPH H$_2$O HCl HCN HNO$_3$ HO$_2$ HOCl IWC IWP N$_2$O O$_3$ OH RHI SO$_2$ T Lvl 3

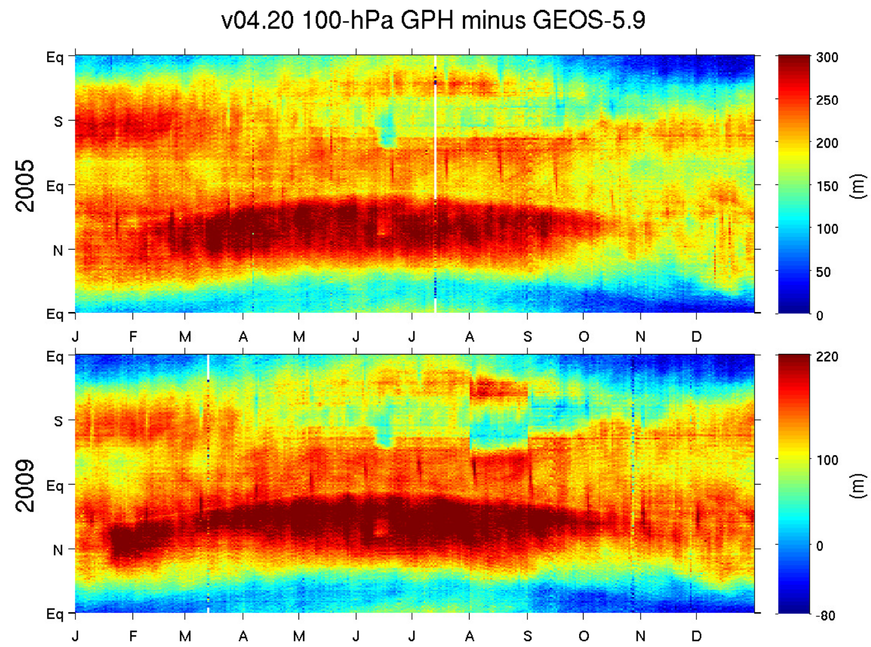

Figure 3.8.3: Daily-binned differences between v4.2x and GEOS-5.9 100-hPa GPH as functions of orbital position. Orbital position, from the bottom of each panel, ascends from the equator to the northern terminator, descends through the equator to the southern terminator and then ascends to the equator.

GEOS-5.12.4 FP-IT, are available in time to be used in routine MLS processing and also provide the temperature *a priori* for the retrieval. At 100 hPa, the model of the near-real-time system is good enough that differences that would accrue by waiting for a reanalysis with additional assimilated data (e.g., MERRA-2) are generally negligible compared to the GPH biases that were present in v4.2*x*.

In v5.0*x*, each profile is offset in height so that the 100 hPa GPH reference level matches that of the GEOS-5. Differences between GEOS-5 GPH and v5.0*x* GPH at other retrieval levels are the accumulated differences between GEOS-5 and MLS temperatures as these differences are integrated (as in Equation 3.1) away from 100 hPa. The 100 hPa GPH produced by the MLS v5.0*x* retrieval, analogous to the 100 hPa GPH level from v4.2*x*, is stored as a diagnostic swath in the "DGG" file before is is overwritten with GEOS-5 values.

3.8.4 Vertical resolution

The GPH profile is vertically-integrated temperature, so its vertical resolution is not well-defined. The vertical resolution of the underlying temperature given in Section 3.22 is repeated in Table 3.8.1.

3.8.5 Precision

MLS v5.0*x* GPH precision is summarized in Table 3.8.1. Precision is the random component of measurements that will average-down if a measurement is repeated. The retrieval algorithms produce an estimate of GPH precision only for the 100 hPa reference level, as this is the only element included in the MLS "state vector." In v5.0*x*, this this level is replaced by the GEOS-5 100 hPa GPH, and so has no random error from MLS radiance noise, leading to the 0 m precision reported for 100 hPa in Table 3.8.1. Precisions at other standard-product profile levels (summarized in column 2 of Table 3.8.1) are calculated from the profiles of temperature precisions. Estimated precisions remain at 20–25 m up to 1 hPa and degrade to 110 m at 0.01 hPa. Off-diagonal elements of the temperature/GPH error covariance matrix are neglected in this GPH-precision-profile calculation, but resulting errors are believed to be small.

3.8.6 Accuracy

The v5.0*x* GPH accuracy has been modeled through consideration of a variety of sources of systematic error, much as v2.2 GPH accuracy was modeled, as discussed in *Schwartz et al.* [2008]. Results of these calculations are given in column four of Table 3.8.1. Substantial biases believed to originate in satellite pointing data and/or time-varying biases in the instrument pointing system have been removed through the use of GEOS-5 100 hPa GPH as an absolute GPH reference rather than information from the satellite attitude and instrument scan model. Of the remaining error sources considered, modeled amplifier non-linearity has the largest impact, just as is the case with the calculation for temperature.

"Observed bias uncertainty" in Table 3.8.1 is an estimate of bias based upon comparisons with analyses and with other previously-validated satellite-based measurements. These comparisons were made using MLS v2.2, but as the biases between v2.2 and v5.0*x* GPH are generally less than 50 m from 261 – 0.1 hPa and reasonably constant, these results hold for v5.0*x* as well. The primary sources of correlative data were the Goddard Earth Observing System, Version 5.0.1 data assimilation system (GEOS-5) [*Rienecker et al.*, 2007], used in the troposphere and lower stratosphere, and the Sounding of the Atmosphere using Broadband Radiometry (SABER) [*Mlynczak and Russell*, 1995], used in the upper stratosphere through the mesosphere. MLS v2.2 has a 150 m high bias relative to analyses (GEOS-5) at 100 hPa that drops to 100 m at 1 hPa. Biases with respect to SABER are small at 0.1 hPa but increasingly negative at higher levels, reaching −600 m at 0.001 hPa, but with significant latitudinal and seasonal variability.

3.8.7 Known Artifacts

GPH of v4.2*x* and earlier versions had large artifacts, reaching ∼3500 m in amplitude, in the orbit following "inclination adjustment maneuvers" (IAMs) done to keep Aura in the "A-Train" constellation of satellites. IAM-related biases are eliminated in v5.0*x* by the use of 100 hPa GEOS-5 GPH as an absolute reference, but the science team will continue to update the list of times when v4.2*x* and earlier versions should be avoided, at least until v4.2*x* processing is discontinued. This list can be found at `https://mls.jpl.nasa.gov/cal/issues.txt`.

3.8.8 Data screening

GPH should be screened in much the same way as is temperature:

Pressure range: 261–0.00046 hPa.

Values outside this range are not recommended for scientific use.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5). GPH precision is set negative at and beyond any level in the integration of temperature away from the 100 hPa reference level where temperature has negative precision.

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Clouds: Thick clouds are believed have some impact on v5.0*x* GPH measurements in the upper troposphere (261–100 hPa). Tropospheric GPH may be screened using the ice water content (IWC) product, rejecting profiles between 261–100 hPa for which the 215 hPa value of IWC is greater than 0.005 g/m^3.

Table 3.8.1: Summary of MLS GPH product.

Region	Resolution Vert. × Horiz. / km	Precision[a] / meters	Modeled accuracy[b] / m	Observed accuracy[c] / m	Comments
<0.00046 hPa	—	—	—	—	Unsuitable for scientific use
0.00046 hPa	13 × 316	±190	4200	—	more validation needed
0.001 hPa	12 × 280	±170	700	450	
0.01 hPa	11 × 250	±110	250	100	
0.1 hPa	6 × 170	±45	250	100	
1 hPa	7 × 165	±20	120	100	
10 hPa	4.1 × 165	±11	30	100	
100 hPa	4.6 × 165	±0	20	20	
261 hPa	3.8 × 167	±8	30	50	
1000–316 hPa	—	—	—	—	Unsuitable for scientific use

[a]Precision on individual profiles
[b]Not including pointing contribution.
[c]Validation is based upon SABER and GEOS-5 comparisons with MLS v2.2 and should be updated.

Quality: Only use profiles with `Quality` greater than 0.2 for the 83 hPa level and smaller pressures, and profiles with `Quality` greater than 0.9 at pressures of 100 hPa and larger.

Convergence: Only profiles whose `Convergence` field is less than 1.03 should be used.

Use of this threshold typically discards less than 0.1% of profiles and is primarily a safeguard against profiles with extremely poor convergence.

3.9 Water Vapor (H_2O)

Swath name: H2O

Useful range: 316–0.001 hPa

Contact: Alyn Lambert (stratosphere/mesosphere), **Email:** <alyn.lambert@jpl.nasa.gov>
William Read (troposphere), **Email:** <william.g.read@jpl.nasa.gov>

3.9.1 Introduction

The standard water vapor product is taken from the 190-GHz “CorePlusR2” retrieval. The vertical grid for H_2O is: 12 levels per decade change in pressure (LPD) for 1000–1 hPa, 6 LPD for 1.0–0.1 hPa, and 3 LPD for 0.1–10^{-5} hPa. The horizontal grid is every 1.5° along the orbit track. H_2O is unusual among MLS products in that it is assumed that the logarithm of the volume mixing ratio (VMR), and not mixing ratio itself, varies linearly with log pressure; however, H_2O, like the other MLS constituents is retrieved in VMR (not log VMR). Vertical and horizontal interpolations of H_2O should be performed linearly on the logarithm of the H_2O concentration (VMR). The concentration of H_2O in the MLS files are unitless, VMR, in the Level 2 Geophysical Product (L2GP) files; however, its concentration is quite low in the upper atmosphere and it is more convenient to express its concentration in parts per million volume (ppmv = VMR$\times 10^6$), a unit commonly used to describe its features in this section. The recommended vertical range is 316–0.001 hPa (height indices, 7–49, starting at 1). The uppermost retrieved level 0.00046 hPa (height index 50) is not vertically resolved from the levels above it and should be regarded as more like a column measurement, but it may be usable for some studies. The MLS science team should be consulted prior to using data from 0.00046 hPa level.

The MLS v5.0*x* H_2O between 1000 and 383 hPa is taken from a retrieval of relative humidity with respect to ice (RHi) product, converted to specific humidity using the Goff-Gratch vapor pressure over ice equation. This RHi retrieval is not vertically resolved, and all levels between 1000 and 383 hPa are assumed to have the same RHi. See Section 3.20 for more information. H_2O for $p \leq 0.000215$ hPa are filled with *a priori* values. Validation of MLS v2.2 water vapor is presented in *Read et al.* [2007] and *Lambert et al.* [2007]. This section reiterates the key information from those studies, and updates them for v5.0*x*. Table 3.9.1 gives a summary of MLS v5.0*x* H_2O precision, resolution, and accuracy.

3.9.2 Changes from v4.2*x*

A defect in v4.2*x* and prior versions is that MLS exhibits a rather low bias (20–50%) at 2–3 km below the tropopause [*Read et al* in prep, 2020]. Another deficiency is that MLS likely underestimates the seasonal cycle at 147 hPa in the tropics. The two issues are related. The tropopause height has a strong seasonal cycle in the tropics and the dry bias at a given height will be modulated accordingly. This has acted to flatten the seasonal cycle at 147 hPa in earlier MLS versions. Finally, it is clear that the MLS H_2O measurement is slowly drifting, due to aging of the instrument. A possible drift in the MLS H_2O was first noted by *Hurst et al.* [2016]. An in depth investigation into potential causes for all these issues has shown the most likely contributors to be a sideband fraction characterization error combined with a radiometer pointing error.

The center channels in the MLS band dedicated to measuring H_2O (band 2) are opaque when the instrument views the stratosphere. Signals in these channels therefore provide a measure of stratospheric temperature. Evaluation of these signals reveals an unexpected offset relative to expectations from observed stratospheric temperatures, and also shows a drift in this offset. This analysis led to a time-dependent correction for the sideband fraction for the 190 GHz receiver (the relative sensitivity to the upper and lower sideband signals, see Section refsec:MLSRadiances). Specifically, the analysis suggests that 190 GHz radiometer lower sideband fraction is 6.85% lower than the value measured pre-launch and has drifted ∼1% during the mission lifetime. Implementing a (time-dependent) correction for the sideband fraction helped resolve another inconsistency with the 190 GHz measurements. Specifically if the H_2O linewidth is used to retrieve pointing (i.e., tangent pressure), the resulting pointing estimates differ from those measured by the 118 GHz and 240 GHz radiometers (which observe O_2 signals) by 250 m at the tangent point. Applying the sideband correction reduced this inconsistency to 70 m, which is within the uncertainty in the radiometer pointing alignment measured prior to launch (and refined based on MLS observations of the moon). Therefore, to further improve this agreement, a 70 m adjustment to the radiometer alignment has also been applied in the v5.0*x* retrievals. With these adjustments the retrieved ptan from the 190 GHz (CorePlusR2) is now consistent within ∼20 m of that retrieved from the 118 and 240 GHz receivers, and is retrieved operationally now. These changes have helped to mitigate the large dry bias 2–3 km below the tropopause, and consequently increased the seasonal cycle of the 147 hPa H_2O in the tropics. These changes have also helped to reduce biases and drifts between the 190 GHz ozone and the ozone from the 240 GHz receiver, which forms the ozone standard product.

Another improvement to the H_2O retrieval in v5.0*x* has been obtained using a fully line-by-line radiative transfer model to calculate radiances for the digital autocorrelator channels (128 channels, each 100 kHz wide, centered on the H_2O line) instead of a simple linear approximate forward model. This change properly accounts for non linearities in the signals' dependence on H_2O concentration. Some adjustments were made to the *a priori* precision and smoothing to improve the precision and potentially make the product useful up to 0.001 hPa. The retrieval range for H_2O has been raised to 0.00046 hPa in v5.0*x*.

The median daily `Quality` metric for v4.2*x* declined by 4.8% over the period from 2010 to 2020. The decline follows a declining trend in the radiometer system temperature that determines the measurement signal noise. The `Quality` metric (a reciprocal of a χ^2-like radiance fit measure) accordingly declines as the fits become worse compared to the expected radiance precision. Inclusion of the tangent pressure retrieval in v5.0*x* has reduced the decline to 0.8%.

Figure 3.9.1 compares MLS v5.0*x* H_2O to that from all previous versions, starting with v2.2. The differences are shown with respect to v2.2 — the version described in the validation papers. Notable differences include the removal of a kink in v2.2 at 32/26 hPa. This kink was caused by a linewidth error and fixed in version v3.3. In v2.2, H_2O was retrieved on a fine 12 LPD grid from the bottom of the retrieval range to 22 hPa. Version 3.3 extended that region up to 1 hPa. Version 4.2 saw improvements in cloud screening and in the lower resolution initial H_2O phase that is used to initialize values and profile shape smoothing for the final high resolution phase. These changes improved agreement with simulated data at the 316–215 hPa levels. The change in sideband fraction in v5 leads to a 5–10% reduction in H_2O in the stratosphere and above. The combined changes in sideband fraction and assumed radiometer alignment results in a moistening of the levels 2 km below the tropopause. Nominally this is 147 hPa in the tropics, 215 hPa at mid-latitudes and 261 hPa at high latitudes. The extremely low values retrieved at 215 hPa at high latitudes seen in previous versions appear to be less dry in v5.

The handling of humidity data at pressures greater than 316 hPa is unchanged from v4.2*x*. Humidity data at pressures greater than 316 hPa are derived from a broad layer relative humidity retrieval (using low limb viewing MLS wing channel radiances) similar to that obtained from NOAA operational humidity sounders such as TOVS. As noted in [*Read et al.*, 2007], the v2.2 H_2O retrievals at pressures larger than 316 hPa were likely to be ∼30% too high, based on comparisons with AIRS. The accuracy of this retrieval is highly sensitive to the transmission efficiency of the MLS optics system. In v4.2*x* the assumed value of the MLS antenna transmission efficiency was adjusted empirically (within the uncertainty range established from MLS calibration) to give better agreement with AIRS in the tropics. In v5.0*x* the N_2 continuum was adjusted (only for this preliminary RHi retrieval phase), to minimize the clear sky cloud induced radiance bias. This retrieval is used as an *a priori* and profile constraint for the

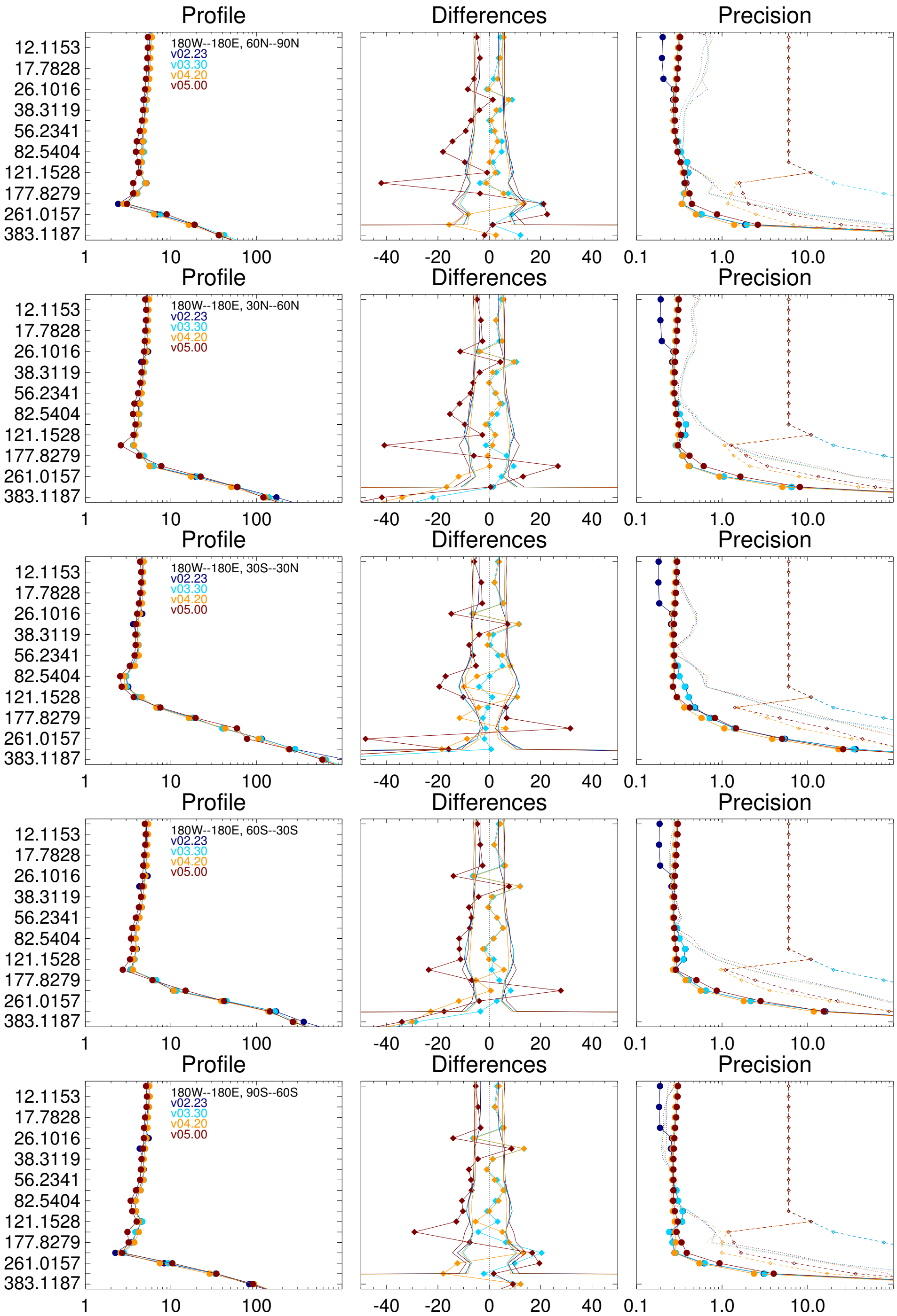

Figure 3.9.1: A comparison of v2.23 (blue), v3.30 (cyan), v4.20 (orange), and v5.00 (red) water vapor for Jan-Feb-Mar 2009 in five latitude bands. X-axes are water vapor mixing ratio in ppmv, y-axes are pressure in hPa. Comparisons for other time periods (not shown) are similar. Left panels compare mean profiles, center panels show the mean differences (red and green diamonds) surrounded by each versions' estimated precision, and right panels show the estimated retrieval precision (solid with bullets), measured variability (dotted, which includes atmospheric variability about the mean), and the a priori precision profile (dashed with small diamonds).

humidity profile at pressures greater than 316 hPa, which are not retrieved in the standard H_2O product retrieval.

The third panel in Figure 3.9.1 shows the mean estimated single profile precision and the measured variability (which includes instrument noise and atmospheric variability). The estimated precisions are similar for most heights. One exception is up high (0.0046–0.00046 hPa), where the smoothing was changed and the uppermost retrieval level raised. Notable changes are also seen in the upper troposphere, where the estimated precision roughly scales by the amount of H_2O. Higher concentrations of H_2O are typically accompanied by larger (i.e., worse) estimates precision error. Taken together, the large dynamic range of possible humidity in the upper troposphere, combined with the non-linear behavior of the instrument response to these concentrations, are the main motivation for choosing a logarithmic representation for H_2O in the retrievals. Differences in precision between v2.2 and later versions result from the use of a coarser retrieval grid above 22 hPa and a different value of the H_2O linewidth.

Figure 3.9.2 compares all versions v2.2 to v5.0*x* over the range from 10 hPa to 0.0001 hPa. As expected, H_2O from v5.0*x* is lower than all other versions except v2.2, which had an erroneous linewidth. Also shown is the increased *a priori* precision being used for v5.0*x* at pressures smaller than 0.0046 hPa, modified in order to make H_2O at the 0.001 and 0.00046 hPa levels usable. Using a non-linear radiative transfer model in v5.0*x*, in place of an approximate linear model for the highly spectrally resolved digital autocorrelator spectrometer (DACS), leads to some differences in the uppermost levels. It is believed that the better model being used for v5.0*x* will produce more accurate results.

Figures 3.9.3 and 3.9.4 show a comparison of H_2O zonal means from v2, v3, v4, and v5 retrievals for 316–8.3 hPa and 6.8–0.00046-hPa, respectively. In the stratosphere, v5.0*x* is usually lower than the previous versions, thanks to the sideband adjustment. Version 5 also shows increased 147 hPa humidity in the tropics, with further increases at 215 hPa in mid latitudes, and yet a more increases at 261 hPa in high latitudes. In the mesosphere $p < 1$ hPa, v5.0*x* H_2O abundances are usually lower than in previous versions but show similar structure up the top level, 0.00046 hPa, where all other versions return the *a priori* (this top level is retrieved in v5.0*x*).

3.9.3 Resolution

The spatial resolution is obtained from examination of the averaging kernel matrices shown in Figure 3.9.5. The vertical resolution for H_2O is in the range 1.3–3.6 km from 316–0.22 hPa and degrades to 6–11 km for pressures lower than 0.22 hPa. The along track horizontal resolution is ~170–350 km for pressures greater than 4.6 hPa, and degrades to 400–740 km at smaller pressures. The resolutions shown in Table 3.9.1 are a summary averages of the equatorial and 70°N values given in Figure 3.9.5. The horizontal cross-track resolution is 7 km, the width of the MLS 190-GHz field-of-view for all pressures. The longitudinal separation of the MLS measurements is 10°–20° over middle and lower latitudes, with much finer sampling in polar regions. The instrument nominally scans to 0.001 hPa, therefore the retrieved value at 0.00046 hPa is not vertically resolved and is effectively a column measurement from 0.001 hPa to the spacecraft, with the H_2O profile values for $p \leq 0.000215$ hPa fixed at *a priori* values.

3.9.4 Precision

Table 3.9.1 summarizes the estimated precision of the MLS v5.0*x* H_2O data. For pressures ≥ 100 hPa, the precisions quoted are the 1σ scatter about the mean of coincident comparison differences, which are larger than the formal retrieval precisions [*Read et al.*, 2007] estimated by the Level 2 software. For $p \leq 83$ hPa the precisions are the 1σ scatter of coincident ascending/descending MLS profile differences [*Lambert et al.*, 2007]. The individual Level 2 precisions are set to negative values or zero in situations when the retrieved precision is larger than 50% of the a priori precision – an indication that the data are biased toward the a priori value.

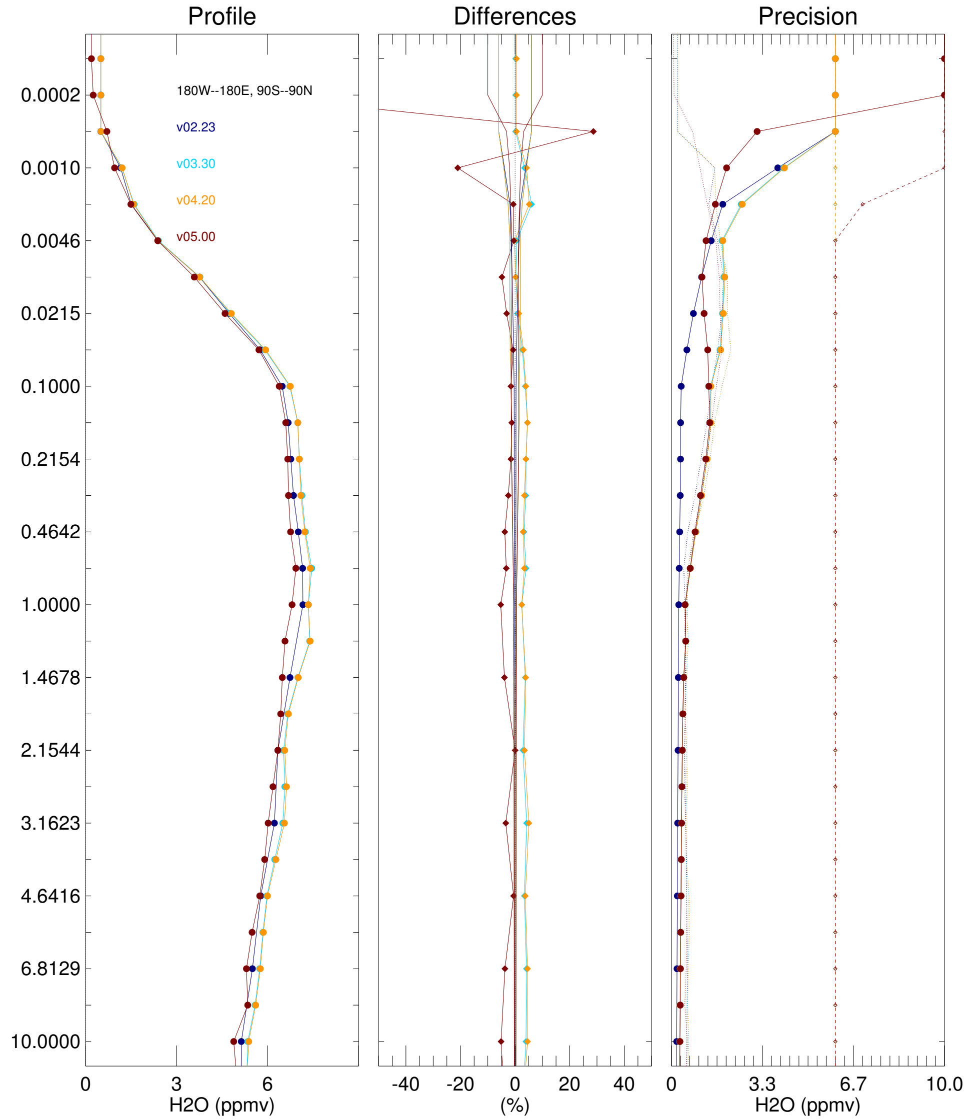

Figure 3.9.2: An all-latitudes comparison of v2.23 (blue), v3.30 (cyan), v4.20 (orange), and v5.00 (red) water vapor for Jan-Feb-Mar 2009 showing levels in the middle stratosphere up to the mesosphere. Other time periods are similar. The left panel compares mean profiles, the center shows the mean difference (red and green diamonds), and the right panel shows the estimated retrieval precision (solid and bullets), measured variability (dotted), which includes atmospheric variability about the mean, and the a priori precision (dashed and small diamonds) profile. Y-axes are pressure in hPa.

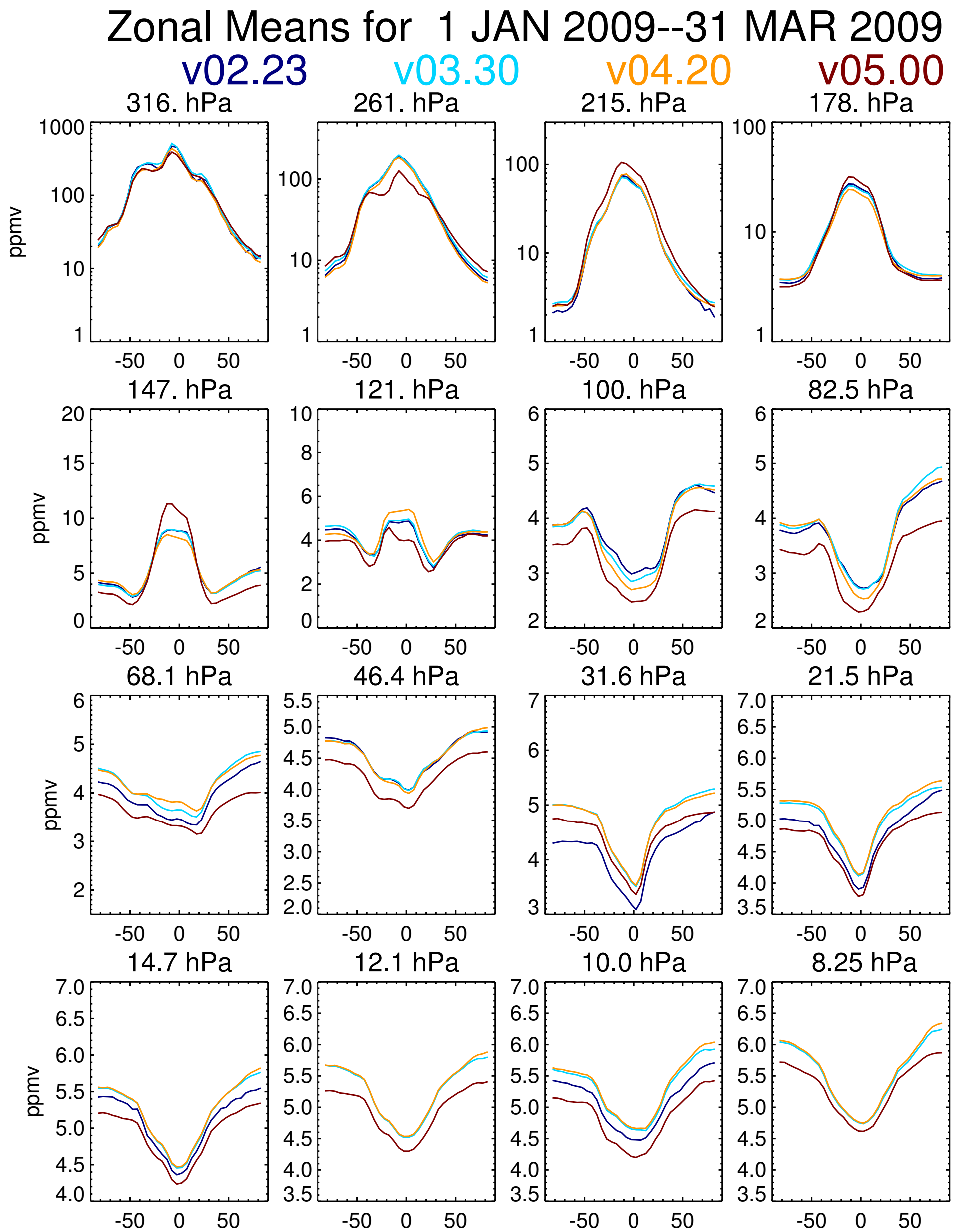

Figure 3.9.3: A comparison of v2.23 (blue), v3.30 (cyan), v4.20 (orange), and v5.00 (red), water vapor zonal means for Jan-Feb-Mar 2009. Each panel represents a pressure as noted above. The pressures shown range from 316 hPa to 8.3 hPa.

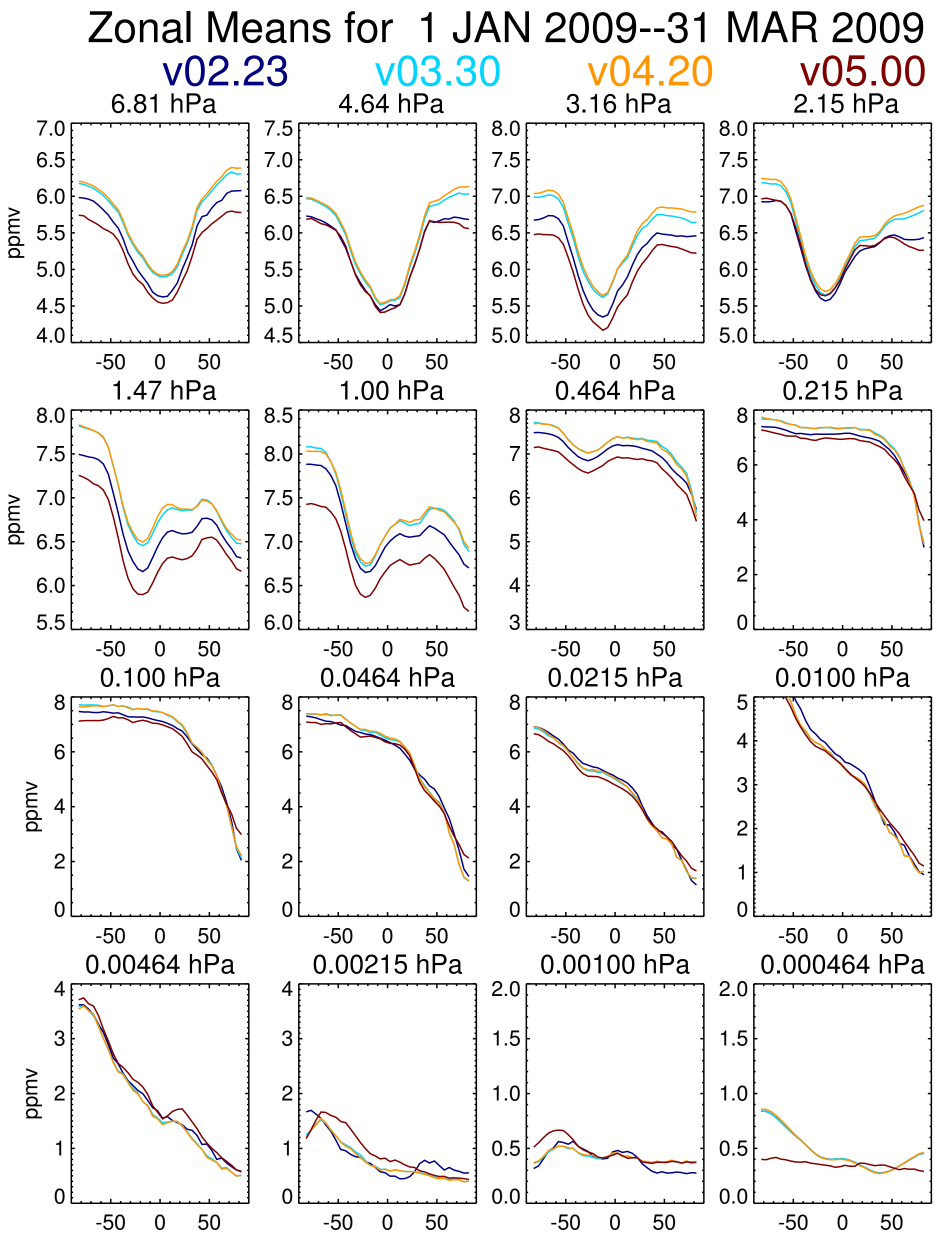

Figure 3.9.4: As Figure 3.9.3 but for 6.8 hPa to 0.00046 hPa.

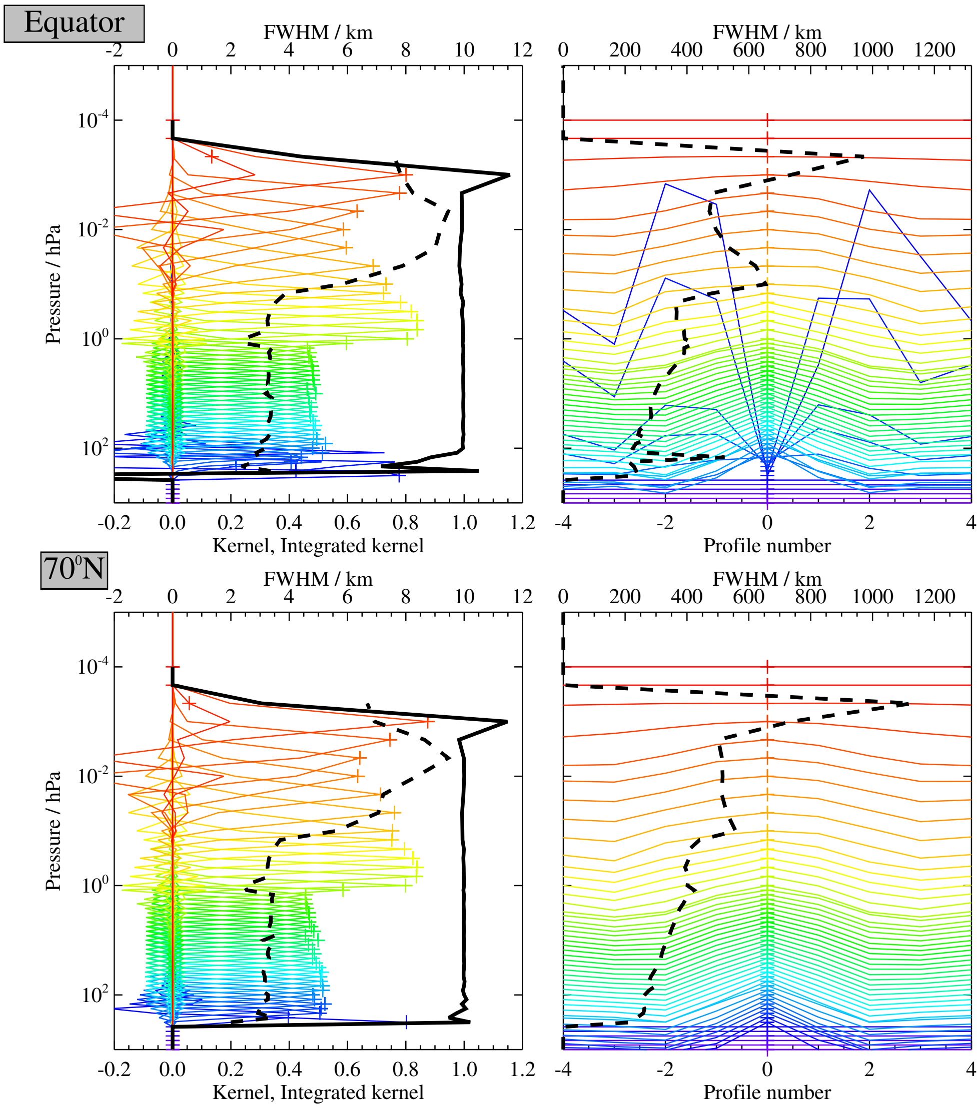

Figure 3.9.5: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x H_2O data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO CH3Cl CH3CN CH3OH ClO CO GPH H2O HCl HCN HNO3 HO2 HOCl IWC IWP N2O O3 OH RHI SO2 T Lvl 3

3.9.5 Accuracy

The values for accuracy are based primarily on two sources: comparisons with other validated instruments and a full systematic error analysis performed on the MLS measurement system as described (for v2) in *Read et al.* [2007] and *Lambert et al.* [2007] (the same approach is planned for v5.0*x*). The results shown in Table 3.9.1 are for v4.2*x* — analysis for v5.0*x* is yet to be performed. However, it is expected that accuracy estimates for v5.0*x* will be similar to those in v4.2*x* repeated here. For pressures between 316 and 178 hPa, comparisons between AIRS v6 and MLS v5.0*x* show < 20% agreement in the zonal mean (with MLS usually drier for low concentrations and wetter for high concentrations) equatorward of 40°, with MLS having a dry biases at higher latitudes.

The values in Table 3.9.1 for pressures between 316 and 178 hPa are drawn from AIRS validated accuracies, which are better than those theoretically possible for the MLS measurement system. For the pressure range 178–83 hPa, the quoted values come directly from the systematic error analysis performed on the MLS measurement system. Comparisons between MLS and frost point hygrometers show that, for v4.2*x*, when the tropopause is between 215 and 147 hPa, MLS H_2O 2–3 km below the tropopause tends to have a large (20–40%) dry bias. It is anticipated that this dry bias will be reduced in v5.0*x*, but this has yet to be fully confirmed in the v5.0*x* data available to date. *[COMMENT: Michelle: This line about whether the dry bias has been reduced in v5 should be updated, and a reference to your ACP paper added.]* The reported accuracy in the 121–83 hPa range is also taken from the systematic error analysis performed on the MLS measurement system. Comparisons among *in situ* sensors on the WB-57 high altitude aircraft and frostpoint hygrometers flown on balloons show 30% disagreements near the tropopause and in the lower stratosphere – well in excess of the estimated accuracy of each instrument, including MLS. The balloon based frost point hygrometer shows agreement better than indicated in Table 3.9.1. The validation paper describes in detail why a 30% spread is inconsistent with the MLS measurements [*Read et al.*, 2007]. For pressures less than 83 hPa, the accuracy is based on the systematic error analysis.

A reported long term drift in H_2O is being addressed in v5.0*x*. It is believed that a drift in the instrument sideband fraction is at least part of the cause. Using opaque signals in the 190 GHz radiometer this sideband fraction drift can be evaluated and corrected. More investigation to assess the performance of this correction is planned.

3.9.6 A note about the water vapor averaging kernels

In general, averaging kernels are most applicable to linear and moderately non-linear retrieval problems. The MLS H_2O retrievals are mostly linear, except when the atmosphere approaches opaqueness. This occurs when the limb tangent of the instrument field of view is less than 10 km above the Earth's surface and the atmosphere is moist. In such cases the measurements are very nonlinear and often times the averaging kernel calculations for the lowest retrieved levels are numerically unstable, and unrepresentative of the actual MLS measurement system. This is the case, for example, for the 316 hPa and 262 hPa equatorial kernels shown in Figure 3.9.5. Analysis of simulated MLS observations indicates that application of the averaging kernel provides little benefit to analyses involving the 316 hPa and 262 hPa levels, and accordingly we recommend not applying the (unrepresentative) kernels at those levels.

3.9.7 Review of comparisons with other datasets

Figure 3.9.6 shows a zonal mean comparison among several satellite data sets including MLS v5.0*x*, AIRS v6, ACE-FTS v3.5, MIPAS IMK v4, HALOE v19, Odin SMR continuum H_2O, and Odin SMR line resolved H_2O. The data sets show agreement for the stratospheric levels shown here beginning with 32 hPa and lower. More significant departures exist amongst them between 121–38 hPa, with some differences in latitudinal structure. Averaging kernels were not applied here because the nominal resolution of these datasets are similar. However, each dataset will exhibit its own vertical smoothing and *a priori*

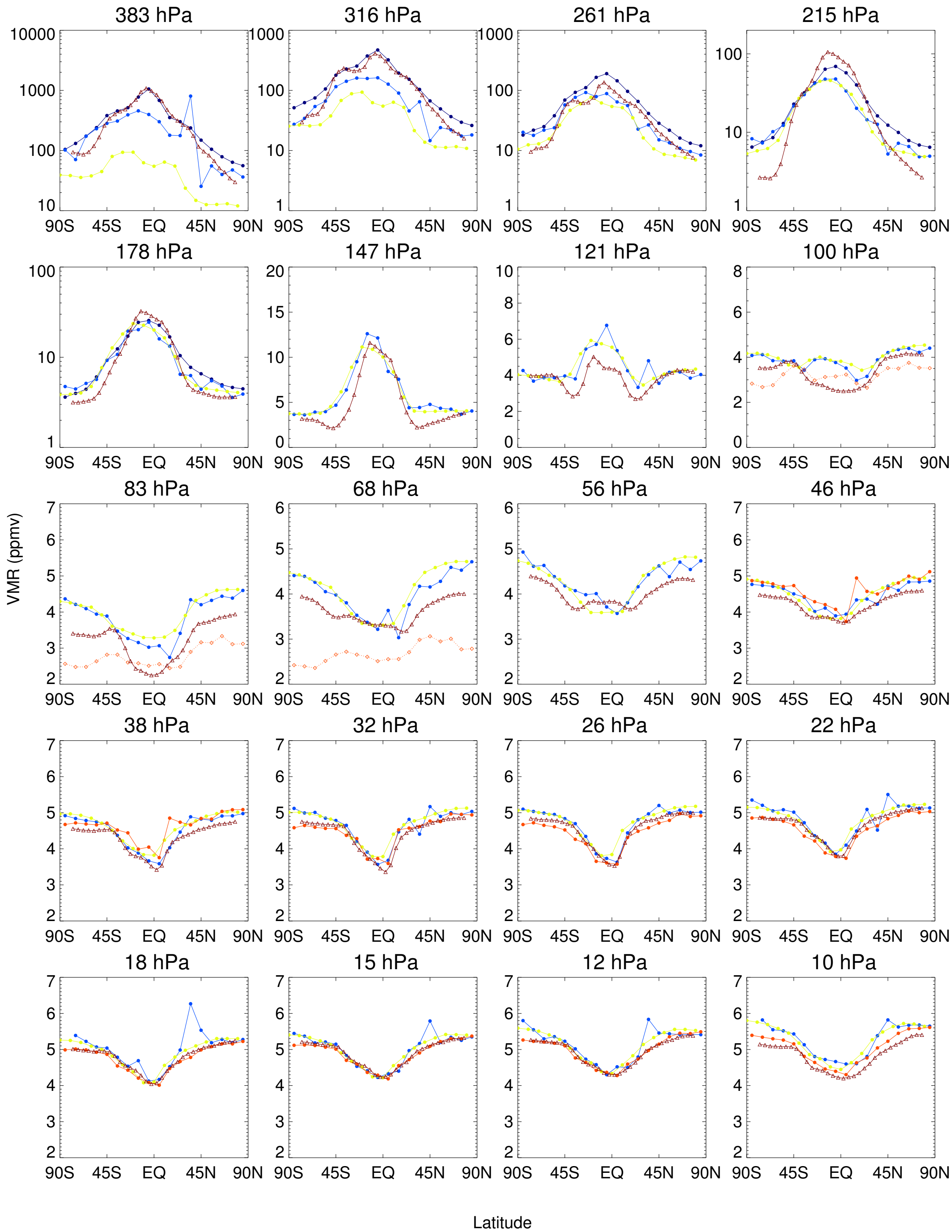

Figure 3.9.6: A comparison of MLS v5.0x (red) water vapor for Jan-Feb-Mar 2009 with other satellite observations shown as latitude-value zonal means. Each panel represents a pressure surface. The satellites are: AIRS v6 (dark blue), ACE-FTS v3.5 (light blue), MIPAS IMK v4 (yellow-green), HALOE v19 (cyan), Odin SMR 544 GHz continuum product (orange open diamonds), and Odin SMR line resolved product (orange solid bullets).

Help Overview Table BrO CH3Cl CH3CN CH3OH ClO CO GPH H2O HCl HCN HNO3 HO2 HOCl IWC IWP N2O O3 OH RHI SO2 T Lvl 3

dependencies that contribute to the differences, particularly where around the tropopause with its sharp vertical gradient. The patterns are more similar for the upper tropospheric levels (316–147 hPa).

One potential improvement in v5.0*x* is shown in Figures 3.9.7 and 3.9.8 that compare multi-month maps of MLS with AIRS v6. The very moist regions over the tropics in v4.2*x* and v5.0*x* are drier than in v2.2 and v3.3 for the higher pressure levels and in better agreement with AIRS.

Apart from the differences noted above, the MLS v5.0*x* H_2O is similar to the v4.2*x*, v3.3, and v2.2 products, the latter described and validated in *Read et al.* [2007] and *Lambert et al.* [2007]. The H_2O validation paper used AIRS v4 and MLS v2 humidities, and both of these data records show reduced humidities in their subsequent versions. A revised validation paper for H_2O is not planned in the near future and users are encouraged to read *Read et al.* [2007] and *Lambert et al.* [2007] for more information. MLS v4.2 is a part of the second SPARC Water Vapor Assessment (WAVAS-II) activity.

3.9.8 Potential drift in lower stratospheric water vapor

Comparisons of lower stratospheric H_2O between MLS and balloon-borne CFH and FPH[1] from 2004 to the present time show a drift in the agreement with MLS water vapor increasing at a rate of 0.03–0.07 ppmv yr^{-1} relative to the frostpoint sondes (roughly 0.6 to 1.5% per year), starting around 2009 *Hurst et al.* [2016]. Comparisons with the ACE-FTS instrument, and with measurements of upper stratospheric water vapor from ground-based microwave sensors, provide evidence for a smaller (∼+0.2% per year) drift. The new calibration values for the sideband fraction that are updated monthly are yet smaller, but approach the drift seen with ACE-FTS. Accordingly, we anticipate that v5.0*x* H_2O will show only a small drift compared to the ACE-FTS record, but continue show a drift compared to the frostpoint record. A complete assessment of the drift correction will have to wait until more of the MLS data are processed to v5.0*x*.

3.9.9 Data screening

Pressure range: 316–0.001 hPa.

Values outside this range are not recommended for scientific use. Data at 0.00046 hPa represents a total column at and above that pressure level. Scientific use of these 0.00046 hPa data may be possible, but requires consultation with the MLS team.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Clouds: Profiles flagged as being affected by high or low clouds (i.e., with `Status` bits corresponding to values of `16` and `32` set) can continue to be used. See artifacts for more details.

Quality field: Only profiles with a value of the `Quality` *greater* than 0.7 should be used in scientific studies.

The quality threshold is deliberately set low because it is not a very good discriminator of poor profiles except when quality is well below the mean value; therefore, we recommend the "additional screening to avoid outliers," as described below.

Convergence field: Only profiles with a value of the `Convergence` *less* than 2.0 should be used in scientific studies.

[1]Cryogenic Frostpoint Hygrometer (CFH) and Frost Point Hygrometer (FPH)

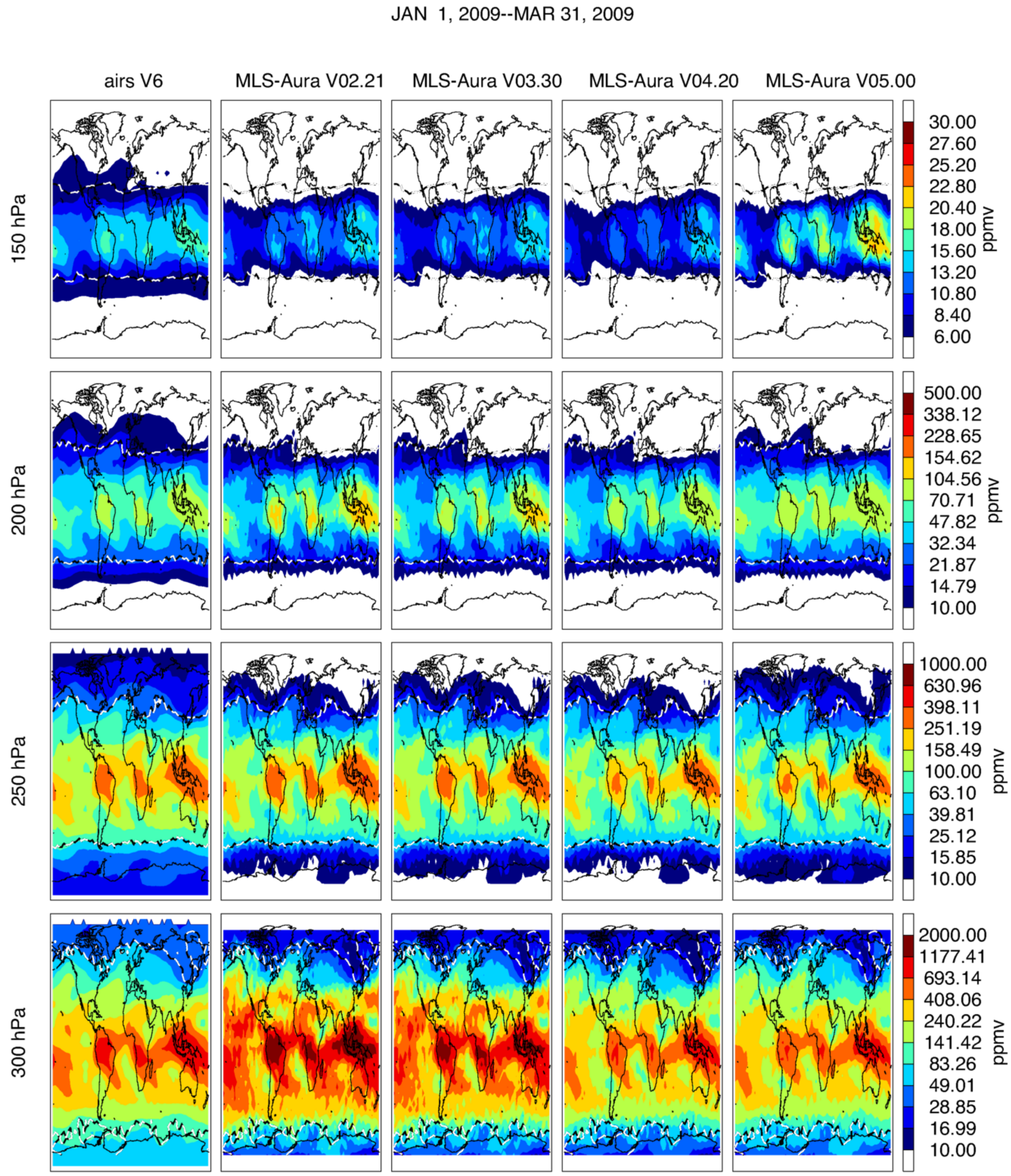

Figure 3.9.7: Mapped fields from AIRS v6 (left), MLS v2.2 (center-left), MLS v3.3 (center), MLS v4.2x (center-right), and MLS v5.0x (right) pressures between 300 and 150 hPa for Jan-Feb-Mar 2009. The black-white lines indicate the tropopause where the region poleward is in the stratosphere. Note that the AIRS measurement is mostly suitable for H_2O greater than 10 ppmv.

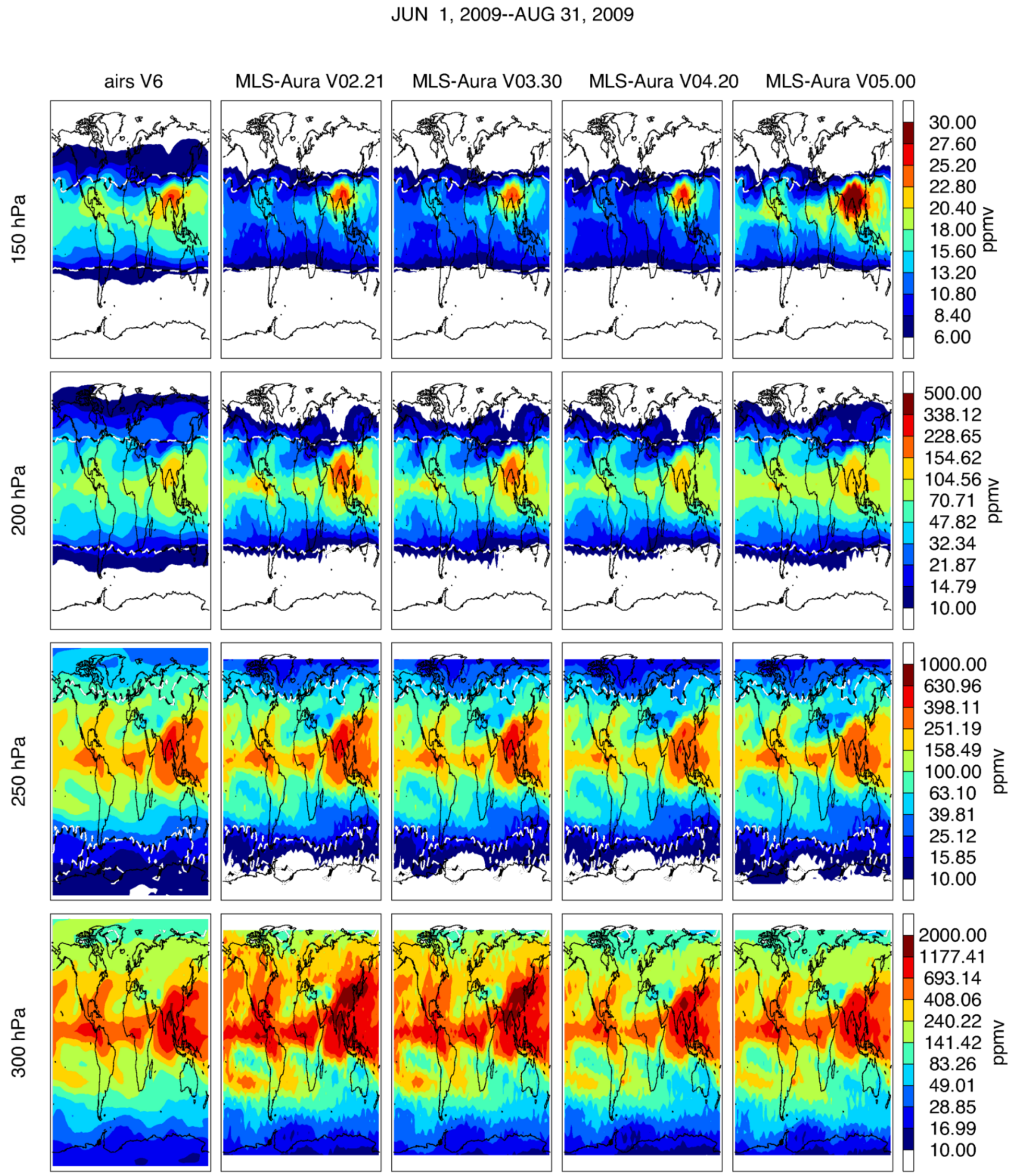

Figure 3.9.8: As Figure 3.9.7 but for Jun-Jul-Aug 2009.

Additional screening to avoid outliers: After application of the `Status`, `Quality`, and `Convergence` screening described above, some unphysical profiles remain in the MLS v5.0*x* H_2O dataset. These are characterized by unrealistically low water vapor mixing ratios in the upper troposphere and stratosphere. The cause behind this behavior is from using the logarithmic basis which excludes negative values. Sometimes the retrieval minimizer seeks a negative value at a given level (which is almost always accompanied by severe vertical profile oscillations). Such values are not allowed and therefore an optimal fit to the measurement signal is not achieved. H_2O profiles having values less than 0.101 ppmv (0.101×10^{-6} VMR) at any pressure at or larger than 1 hPa (vertical levels 1–37) should not be used. Profiles with acceptable `Status`, `Quality`, and `Convergence` having values less than 0.101 ppmv at pressures $<$ 1 hPa (vertical levels 38–55) are acceptable and occur frequently, because the water vapor concentration in the mesosphere is often less than the measurement precision and negative values are preferable but not realizable due to the logarithmic basis definition being used.

3.9.10 Artifacts

There is a minimum concentration where MLS H_2O measurements become unreliable. This is given in Table 3.9.1 under the "Min. H_2O" column. The lowest allowable H_2O value is 0.1 ppmv. Differences between the retrieved middle tropospheric H_2O constraint and the true atmospheric state can cause errors at 316 and 261 hPa. The error manifests either as dry ($<$ 1 ppmv) or moist spikes in an orbital time series. Such data are often accompanied with good quality and status but is rejected by checking the profile for such events.

Clouds in the field of view degrade the data in unpredictable ways. Many instances of quality $<$ 0.7 occur in the presence of clouds where the cloud screening of the radiances failed to reject them. Cloud radiative scattering distorts the spectral lineshape causing poor fits and low quality values. However, not all MLS signals are obviously affected. Coincident comparisons of MLS cloud flagged H_2O (`Status` bits corresponding to values of `16` or `32` set between 316–215 hPa) having good quality with AIRS show a small mean bias of 10% but exhibit a 50% increase in variability for the individual differences. Users should therefore be aware that, although the overall biases for measurements inside clouds are similar to that for clear sky, individual profiles affected by cloud will exhibit greater variability about the true atmospheric humidity than those not marked as being cloud-influenced.

The 190 GHz radiometer signals due to aging are drifting. This drift manifests as a change in the sideband fraction. v5.0*x* makes an attempt to correct this.

In the mesosphere, the precision is often larger than the retrieved value and therefore negative concentrations are possible and proper. The logarithmic definition of the H_2O basis doesn't allow retrieval of negative values, with the minimum lowest allowed concentration being 0.1 ppmv. Therefore an average of many profiles will produce a positive bias. It is recommended that a better representation of the average of many profiles is achieved by calculating its median.

The instrument scan nominally tops out at 0.001 hPa. Therefore, the 0.00046 hPa, which is now retrieved in v5.0*x*, is not a vertically resolved measurement but rather a column amount from 0.001 hPa to the spacecraft, under the constraint that all levels above 0.00046 hPa are fixed at *a priori* values. Accordingly, should there be a large H_2O event in any level above 0.00046 hPa, it would be retrieved as an enhancement at 0.00046 hPa, but its true vertical location above 0.00046 hPa would be unknown.

3.9.11 Desired improvements for future data version(s)

While many defects in v4.2 and earlier versions have been addressed, further investigation of their effectiveness, especially the drift reduction and high latitude low value retrievals in the upper troposphere needs to be undertaken, and improvements made if necessary. It may be possible to obtain a vertically resolved H_2O product for pressure $>$ 316 hPa at high latitudes during dry conditions.

Table 3.9.1: Summary of MLS v5.0x H_2O product.

Pressure / hPa	Resolution V×H / km	Precision[a] / %	Accuracy / %	Min. / ppmv[b]	Comments
≤0.00022	—	—	—	—	Unsuitable for scientific use
0.0005	NVR[c] × TBD	1210	TBD[d]	0.1	Nominally a slant column measurement for p ≤ 0.001 hPa.
0.001	7.1 × 650	973	38	0.1	
0.002	7.8 × 430	417	41	0.1	
0.005	9.4 × 340	127	22	0.1	
0.010	8.3 × 310	60	15	0.1	
0.022	7.3 × 300	39	16	0.1	
0.046	7.0 × 250	28	16	0.1	
0.10	4.8 × 210	20	13	0.1	
0.22	3.3 × 200	17	10	0.1	
0.46	3.2 × 200	12	8	0.1	
1.0	2.5 × 270	6	6	0.1	
2.2	3.6 × 260	6	6	0.1	
4.6	3.5 × 245	5	6	0.1	
10	3.6 × 240	5	19	0.1	
22	3.8 × 220	6	7	0.1	
46	3.8 × 210	6	5	0.1	
68	3.7 × 185	6	8	0.1	
83	3.6 × 185	7	7	0.1	
100	3.5 × 190	7	7	0.1	
121	3.5 × 200	7	17	0.1	
147	3.1 × 200	7	13	0.1	
178	3.3 × 205	6	13	3	
215	2.8 × 205	6	17	3	Extent of a low bias for latitudes > 60° to be investigated.
261	2.8 × 190	7	24	4	Extent of low bias for latitudes > 60° to be investigated.
316	2.3 × 190	16	35	7	Occasionally erroneous low value < 1 ppmv and high value fliers are retrieved in the tropics, usually in clouds.
> 316	—	—	—	—	Unsuitable for scientific use

[a] Precision for a single MLS profile
[b] Minimum H_2O is an estimate of the minimum H_2O concentration measurable by v5.0*x* MLS.
[c] Not Vertically resolved (NVR)
[d] Not yet determined

3.10 Hydrogen Chloride (HCl)

Swath name: `HCl`

Useful range: 100–0.32 hPa

Contact: Lucien Froidevaux, **Email:** <Lucien.Froidevaux@jpl.nasa.gov>

3.10.1 Introduction

There has been very little change in the v5.0*x* HCl retrieval results, in comparison to v4.2*x*. We provide below sample mean HCl distributions for the two data versions, and their differences. Otherwise, previous information regarding this species remains largely unchanged; the main points are mentioned here mainly for new data users.

The MLS v5.0*x* retrievals of the HCl standard product (from the 640 GHz radiometer) use channels from band 14, as a result of the deterioration observed since early 2006 in nearby band 13, originally targeted (with narrower channels than band 14) at the main HCl emission line center. Full measurement days with band 13 on after February 15, 2006, are as follows: March 15, 2006 (2006d074), April 14, 2006 (2006d104), January 6 through 8, 2009 (2009d006 through 2009d008), and January 24 through 27, 2010 (2010d024 through 2010d027). For days prior to February 16, 2006 and for the few days (as listed above) when band 13 gets turned on thereafter, the MLS Level 2 software also produces a separate `HCl-640-B13` product (stored in the `L2GP-DGG` file), using the band 13 radiances. This product has slightly better precision and vertical resolution in the upper stratosphere than the standard HCl product. The MLS team plans to turn band 13 on very infrequently (possibly only one more time), as its lifetime is estimated at a few days to a few weeks at most, based on the channel counts and channel noise characteristics observed during the 3-day turn-on period in late January, 2010; band 13 should provide useful trend information for upper stratospheric data, given its narrower channels. Upper stratospheric trends from the (uninterrupted from 2004 to present) band 14 retrievals are not reliable enough and are too small, compared to band 13 data and expectations, as well as versus ACE-FTS HCl data. Scientific usage of the MLS standard HCl (band 14) dataset should therefore be restricted to the lower stratosphere; in this region, studies of tendencies and longer-term trends are justified (e.g., see the HCl comparisons discussed by *Mahieu et al.* [2014]).

See Figure 3.10.1 for an illustration of the trend differences between these two MLS band measurements of HCl. In the lower stratosphere, however, variations in the two HCl products are closer together, although there is also more seasonal variability. We believe that the band 14 retrievals are quite appropriate to use in studies of seasonal (and latitudinal) changes (e.g., during polar winter/spring), and for longer-term trend studies in the lower stratosphere, despite some systematic trend differences with respect to some model results, as discussed by *Froidevaux et al.* [2019].

Table 3.10.1 summarizes the MLS HCl resolution, precision, and accuracy estimates as a function of pressure. More discussion and data screening recommendations for the MLS HCl v5.0*x* data are provided below. Analyses describing detailed validation of the MLS (v2.2) product and comparisons with other data sets are described in *Froidevaux et al.* [2008a]. Based on the fairly small overall changes in HCl data since v2.2, the conclusions of the latter reference should remain essentially unchanged.

3.10.2 Changes from v4.2*x*

There were no significant algorithmic changes relating to HCl for the v5.0*x* retrievals. Small differences in HCl abundances (see below) have occurred mainly in the bottom part of the lower stratosphere, mainly as a result of changes in retrieved MLS water vapor in the UTLS.

The background observed in the 640-GHz radiances includes emissions from N_2, O_2, and H_2O. There are laboratory-based and ground-based models for the continuum absorptions that are the basis for the

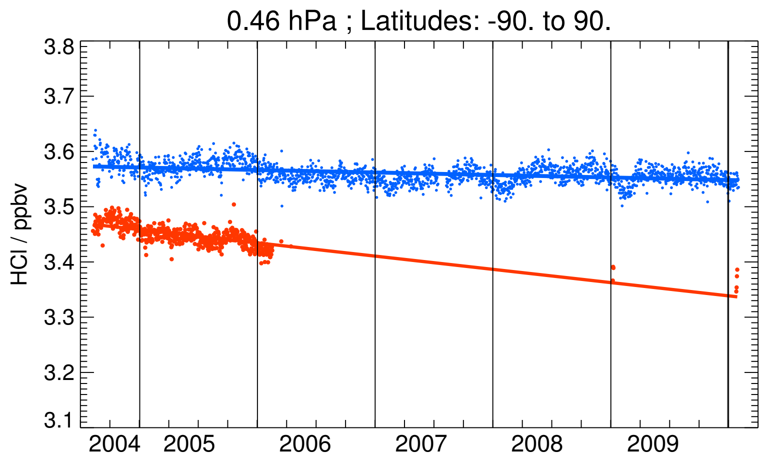

Figure 3.10.1: Daily zonal averages for MLS HCl at 0.46 hPa, from mid-August, 2004, through January, 2010, for the originally-targeted band 13 measurements (red points), now available only on occasion (to preserve lifetime), and the band 14 data (blue points). The lines are simple linear fits through the daily data points; trend differences are apparent in this region of the atmosphere, where the information obtained from band 14 HCl data is not reliable enough.

MLS absorption model [*Pardo, 2001*, and references therein]. These models were tested against MLS extinction measurements from the wing channels in the 640-GHz radiometer. The latitude dependence of this extinction was found to agree better with the expected moist plus dry continuum extinction values if the dry and moist continuum functions were scaled by factors close to 20%; however, this is not a change from the v4.2*x* retrievals.

A comparison plot showing zonal average HCl profile contours versus latitude and differences between the v5.0*x* and v4.2*x* fields for a typical month (March, 2009) is provided in Figure 3.10.2. For pressures larger than or equal to 0.22 hPa, the average differences between the two data versions are typically within 0.05 ppbv (or 1–2%). These average changes are easily within the estimated accuracy values (see Table 3.10.1). The largest percentage changes in HCl occur for very small mixing ratio values; v5.0*x* values are larger than v4.2*x* values by a few to 25% in the 100 to 68 hPa region, and also (not shown here) in the polar lower stratospheric regions during winter/spring. There is still an unrealistic high bias in HCl at 147 hPa in the tropics, so values at this pressure are not recommended or reliable within the 40°S to 40°N latitude range. The precision (single profile random uncertainty) estimates provided in the Level 2 files are essentially unchanged from v4.2*x*.

3.10.3 Resolution

Typical (rounded off) values for resolution are provided in Table 3.10.1. Based on the width of the averaging kernels shown in Figure 3.10.3, the vertical resolution for the standard HCl stratospheric product is ~3 km (2.7 km at best in the lower stratosphere), or about double the 640-GHz radiometer vertical field of view width at half-maximum; the vertical resolution degrades to 4–6 km in the lower mesosphere. The along-track resolution is ~200 to 350 km for pressures of 2 hPa or more, and ~500 km in the lower mesosphere. The cross-track resolution is set by the 3 km width of the MLS 640-GHz field of view. The longitudinal separation of MLS measurements, set by the Aura orbit, is 10°–20° over middle and lower latitudes, with much finer sampling in polar regions.

3.10.4 Precision

The estimated single-profile precision reported by the Level 2 software varies from ~0.2 to 0.6 ppbv in the stratosphere (see Table 3.10.1), with poorer precision obtained in the lower mesosphere. These precision values have not changed significantly for v5.0*x* data. The Level 2 precision values are often only

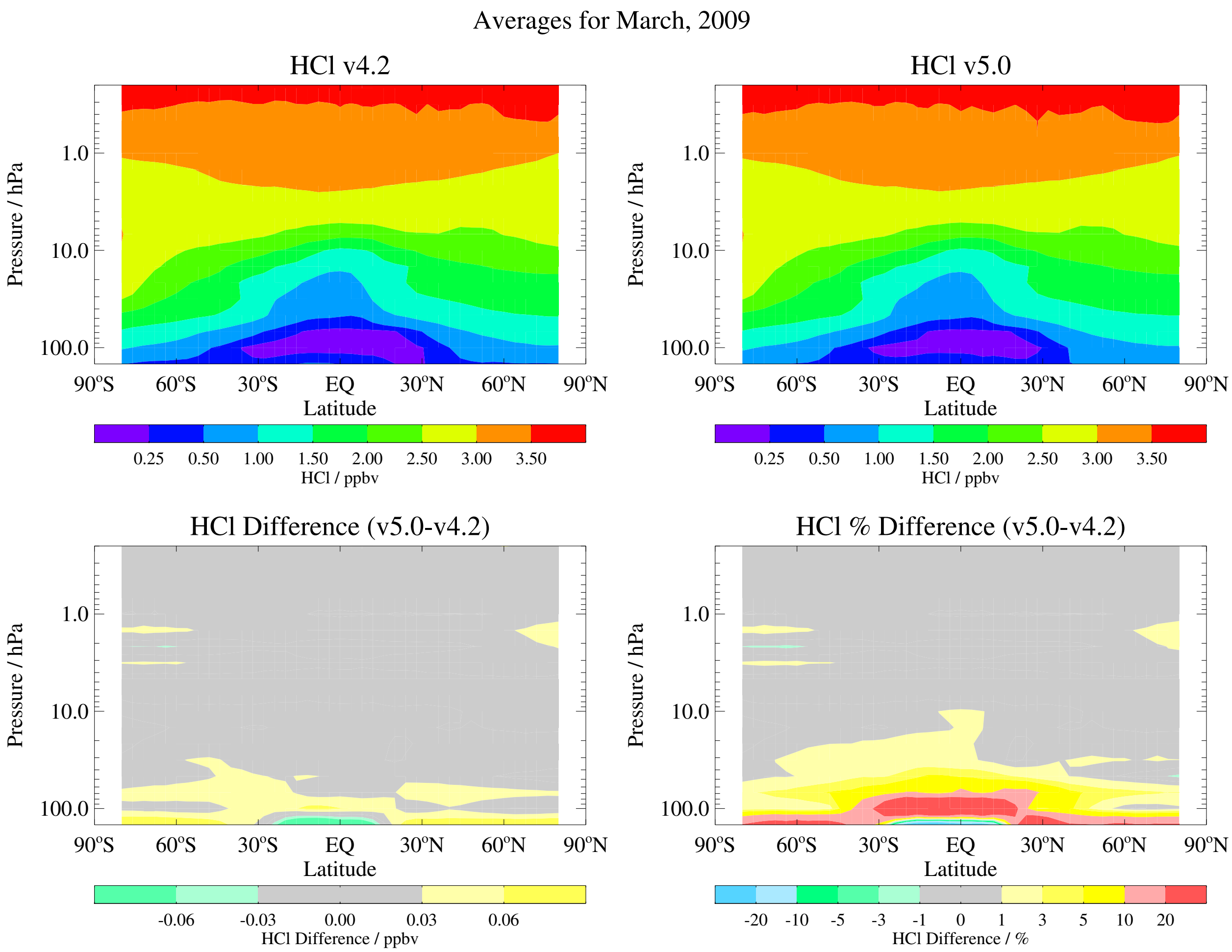

Figure 3.10.2: Zonal averages for MLS HCl profiles during March, 2009, showing the MLS v4.2x HCl mixing ratio contours (top left panel), the v5.0x contours (top right panel), and their differences in ppbv (v5.0x minus v4.2x, bottom left panel) and percent (v5.0x minus v4.2x versus v4.2x, bottom right panel).

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

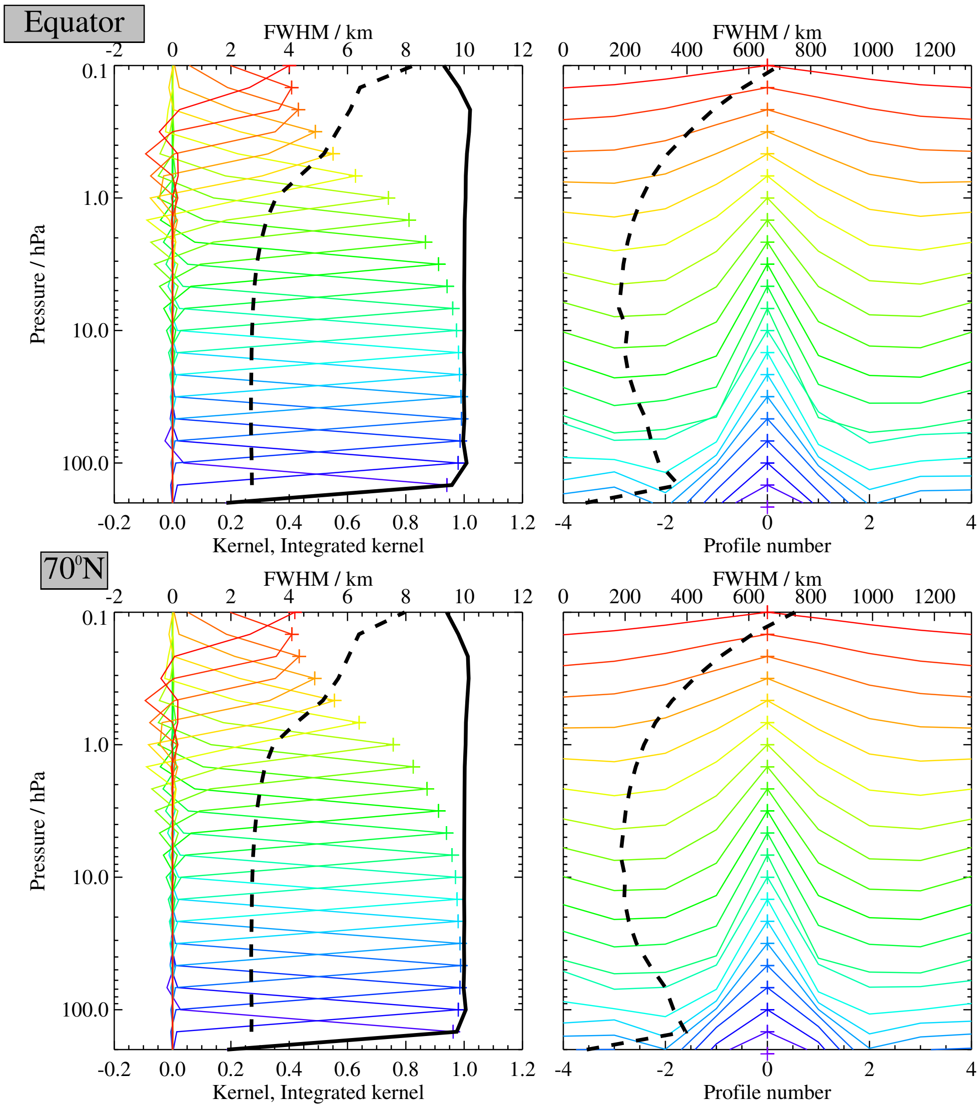

Figure 3.10.3: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x HCl data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

slightly lower than the observed scatter in the data, as evaluated from a narrow latitude band centered around the equator where atmospheric variability is often smaller than elsewhere, or as obtained from a comparison between ascending and descending coincident MLS profiles. The scatter in MLS data and in simulated MLS retrievals (using noise-free radiances) becomes smaller than the theoretical precision (given in the Level 2 files) in the upper stratosphere and mesosphere, where there is a larger impact of *a priori* and smoothing constraints. The HCl precision values increase rapidly at pressures less than 0.2 hPa, and are generally flagged negative (or zero) at pressures less than 0.1 hPa; this indicates an increasing influence from the *a priori* (with poorer measurement sensitivity and reliability).

3.10.5 Accuracy

The accuracy estimates in the Table come from a quantification of the combined effects of possible systematic errors in MLS calibration, spectroscopy, etc. on the HCl retrievals (based on version 4, for now); there are several error sources (mostly from radiometric calibration components) that contribute significantly to the total error. These values are intended to represent 2σ estimates of accuracy. For more details, see the MLS validation paper by *Froidevaux et al.* [2008a]. For v5.0*x* (as for v4.2*x*), given the trend issues affecting the (band 14) standard HCl product in the upper stratosphere and lower mesosphere, we have recommended an accuracy estimate of no better than 10% in this region (or about 0.3 ppbv). For the lower stratosphere, given the agreement between the two bands' retrievals as well as some trend studies (for the standard product), we use the more formal accuracy estimates (see Table 3.10.1). The changes in the accuracy estimates in this Table are typically very small, except at the 147 hPa level, where there are now larger systematic errors.

3.10.6 Data screening

Pressure range: 100–0.32 hPa

Values outside this range are not recommended for scientific use. We note that the MLS values at 147 hPa are biased high, at least at low to mid-latitudes – and these values are not recommended (particularly equatorward of about 40°). Also, although the vertical range at the top end is recommended up to 0.32 hPa, users should note the significant issues relating to HCl trend estimates in the upper stratosphere and lower mesosphere; average profiles in this region can be used for studies not involving trends (or accuracy requirements not as tight as 10%).

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality field: Only profiles with a value of the `Quality` field *greater* than 1.2 should be used.

This criterion removes profiles with the poorest radiance fits, typically less than 0.1% of the daily profiles. For HCl (and for other 640 GHz MLS products), this screening correlates well with the poorly converged sets of profiles (see below); we recommend the use of both the `Quality` and `Convergence` fields for data screening.

Convergence field: Only profiles with a value of the `Convergence` field *less* than 1.05 should be used.

For the vast majority of profiles (99% or more for most days), this field is less than 1.05. Nevertheless, on occasion, sets of profiles (typically one or more groups of ten profiles, retrieved as a "chunk") have this `Convergence` field set to larger values, and should be discarded.

Clouds: Thick clouds can add significant artifacts (mainly in the tropics, statistically), with total systematic errors potentially as large as 0.5 ppbv at 100 hPa and even larger at 147 hPa. Studies in this region could benefit from additional screening that correlates any outliers in the data with the occurrence of thick clouds (using some subset of the profiles with set cloud status flags, namely status bits 16 and 32, or using the MLS retrievals of ice water content). However, the large positive HCl bias at 147 hPa for low latitudes likely arises in part from unknown or improperly modeled systematic error sources, and not just from clouds. At other pressures, the potential impact on HCl from clouds is small or negligible.

3.10.7 Review of comparisons with other datasets

Froidevaux et al. [2008a] provided results of generally good comparisons between MLS HCl and other satellite, balloon, and aircraft measurements. Both MLS and ACE-FTS HCl values are generally larger (by about 10–15%) than the HCl values from HALOE, especially at upper stratospheric altitudes; this feature has not changed, overall, with the new data version(s) from both MLS and ACE-FTS. MLS HCl at 147 hPa is biased high versus WB-57 aircraft in-situ (CIMS) measurements (low to mid-latitudes); while this is still true for v4 data, MLS data at this pressure level are potentially useful and accurate enough at high latitudes.

3.10.8 Artifacts

- We do not recommend the use of the MLS HCl standard product in the upper stratosphere and lower mesosphere, especially in terms of trend studies, for reasons mentioned above.
- The HCl values at 147 hPa are biased high and generally not usable (except possibly at high latitudes). Please consult with the MLS team for further information.
- Users should screen out the non-converged and poorest quality HCl profiles, as such profiles (typically less than 0.1% of the data) tend to behave unlike the majority of the other MLS retrievals. See the criteria listed above.

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

Table 3.10.1: Summary for MLS hydrogen chloride

Pressure	Precision[a]		Resolution V × H	Accuracy[b]		Comments
hPa	ppbv	%	km	ppbv	%	
0.22–0.001	—	—	—	—	—	Unsuitable for scientific use
0.32	0.8	25	5 × 400	0.3	10	Unsuitable for trend studies
0.5	0.7	20	5 × 350	0.3	10	Unsuitable for trend studies
1	0.5	15	4 × 250	0.3	10	Unsuitable for trend studies
2	0.4	15	3 × 200	0.3	10	Unsuitable for trend studies
5	0.3	10	3 × 200	0.3	10	Unsuitable for trend studies
10	0.2	10	3 × 200	0.2	10	
20	0.2	15	3 × 200	0.15	10	
46	0.2	10 to > 40	3 × 250	0.2	20	
68	0.2	15 to > 80	3 × 300	0.2	25	
100	0.3	30 to > 100	3 × 350	0.2	40–45	
147	0.4	50 to > 100	3 × 400	0.5	$\gtrsim$ 100	High bias at low lats. (use with caution elsewhere)
1000–215	—	—	—	—	—	Unsuitable for scientific use

[a] Precision (1σ) for individual profiles; note that % values tend to vary strongly with latitude in the lower stratosphere.

[b] 2σ estimate from systematic uncertainty characterization tests (but see text for estimates at pressures lower than 10 hPa); note that percent values tend to vary strongly with latitude and season in the lower stratosphere, due to the variability in HCl.

3.11 Hydrogen Cyanide (HCN)

Swath name: `HCN`

Useful range: 21–0.1 hPa

Contact: Hugh C. Pumphrey, **Email:** <Hugh.Pumphrey@ed.ac.uk>

3.11.1 Introduction

HCN is retrieved from bands encompassing, in the lower sideband, the 177.26 GHz spectral line of HCN. Although the target line is in an uncluttered part of the spectrum, the upper sideband contains many interfering lines of O_3 and HNO_3. As a result, the v5.0*x* HCN product is not recommended for general use at altitudes below 21 hPa. In the recommended range it is usable, but has rather poor precision (necessitating averaging such as weekly zonal means) and resolution.

It is possible to retrieve weekly zonal means of HCN over a greater vertical range by first averaging the radiances. Results of this process and further information on the HCN measurement may be found in *Pumphrey et al.* [2006].

3.11.2 Differences between earlier versions and v5.0*x*

No changes specific to the HCN retrieval were made between v2.x and v3.x. For v4.x a new phase was introduced in which HCN is retrieved using only bands 6 and 27, rather than all of R2; this phase is also used in v5.0*x*. The v4.x HCN had obvious biases in the lower stratosphere, but they were far less severe than in v2.x and v3.x, both of which had large regions with negative mixing ratios. In v5.0*x* the biases appear to be reduced again. Between 10 hPa and 3 hPa, v5.0*x* HCN is somewhat lower than all three previous versions. The lowest recommended level for v5.0*x* is currently 21 hPa, as it was for v4.x. However, it is possible that, after further validation work, the v5.0*x* HCN data between 31 hPa and 68 hPa may ultimately be judged to be suitable for scientific use. Any such updates will be reported in a new version of this document.

Figure 3.11.2 shows that the precisions in v5.0*x* are essentially unchanged from earlier versions. The retrieved mixing ratios change very little in the region where use was recommended for earlier versions. Mixing ratios are considerably different between all four versions in the lower stratosphere. However, the values in v5.0*x* appear less unrealistic than in any earlier version.

3.11.3 Vertical resolution

The HCN signal is rather small, so a rather strong smoothing constraint has to be applied to ensure that the retrieval is at all useful. As Figure 3.11.1 shows, the vertical resolution is about 8 km at 10 hPa, degrading to 12 km at 0.1 hPa. The horizontal resolution along the measurement track is between 2 and 4 profile spacings.

3.11.4 Precision

Figure 3.11.2 shows the estimated precision (values of the field `L2gpPrecision`), together with the observed standard deviation in an equatorial latitude band where the natural variability of the atmosphere is small. The observed scatter is smaller than the estimated precision due to the effects of retrieval smoothing.

3.11.5 Accuracy

The accuracy of the HCN product has not been assessed in detail because a cursory inspection revealed that v2.x and v3.x HCN had extremely large systematic errors in the lower stratosphere. These errors

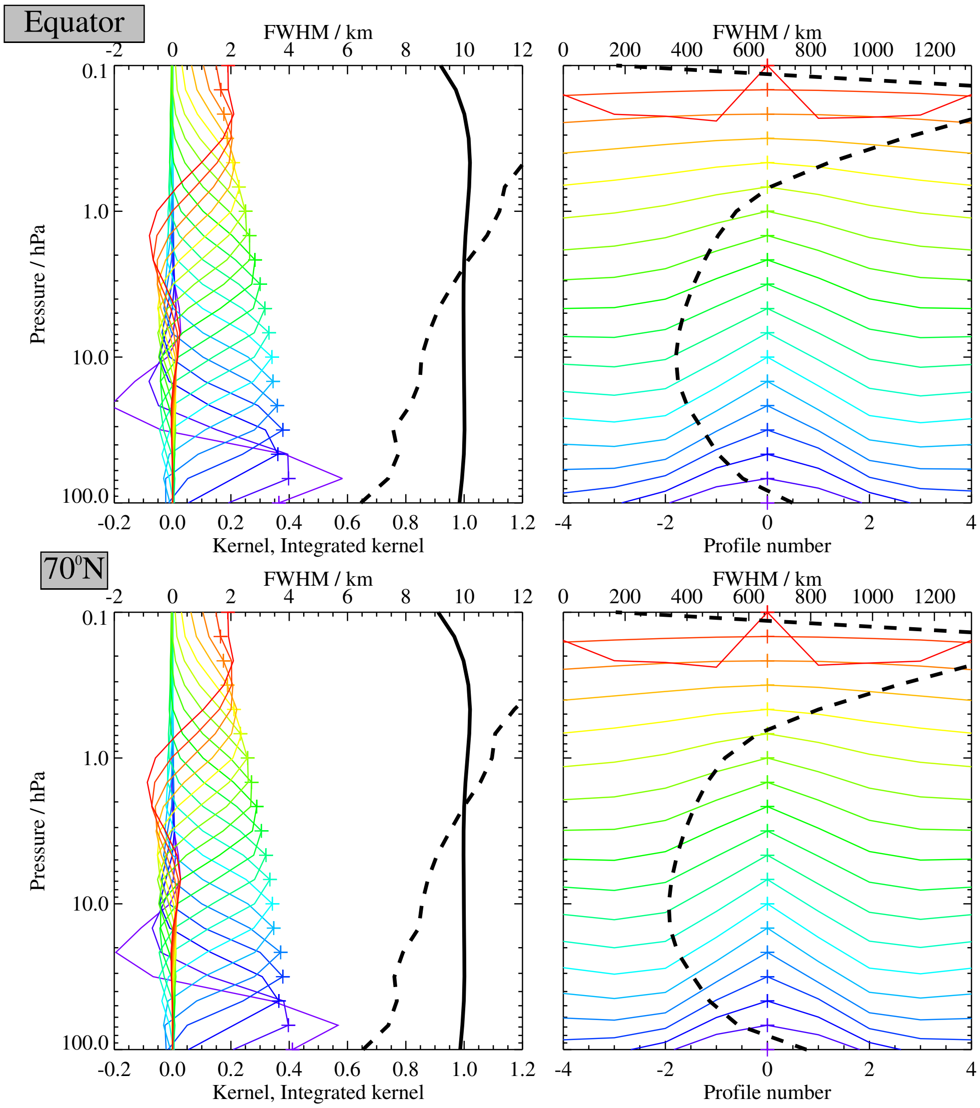

Figure 3.11.1: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x HCN data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

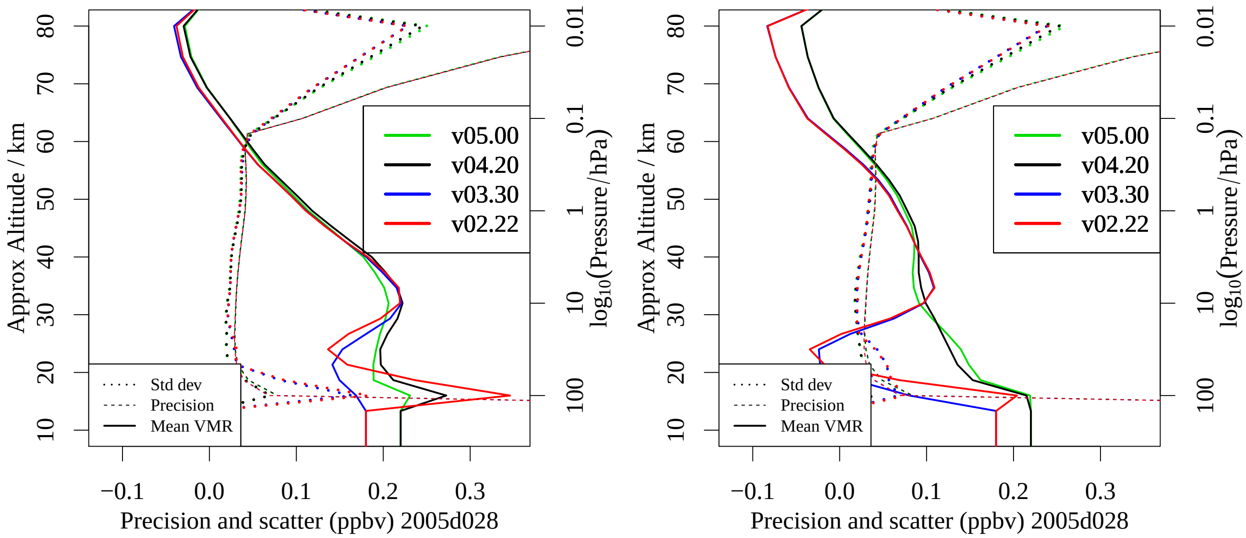

Figure 3.11.2: Estimated precision `L2gpPrecision` and observed standard deviation for MLS v5.0x (green), v4.x (black), v3.x (blue) and v2.x (red) HCN. The data shown are all profiles within 20° of the equator (left) and 70°N–83°N (right) for 28 January, 2005. Mean mixing ratio (VMR) profiles are shown for comparison. Between 3 and 10 hPa, v5.0x departs from the three earlier versions. At altitudes below 10 hPa, all four versions are different, but v2.x and v3.x are less realistic than v4.x and v5.0x.

Table 3.11.1: Summary of data quality for MLS v5.0x HCN. The precision shown is the estimated precision (`L2gpPrecision`); the observed scatter is about 80% of this value.

Pressure	Resolution V × H / km	Precision / pptv	Accuracy / %	Comments
< 0.1 hPa	—	—	—	Unsuitable for scientific use
1–0.1 hPa	12 × 500	50	50	
21–1 hPa	10 × 300	30	50	
100–21 hPa	10 × 300	50	Very poor	Unsuitable for scientific use
> 100 hPa				Not Retrieved

are much smaller in v4.x and may be somewhat smaller again in v5.0*x*, but remain present and unquantified. For this reason the data are not recommended for general use at pressures greater than 21 hPa (altitudes below ∼27 km). In the upper stratosphere the values are in line with current understanding of the chemistry of HCN. Comparison to historical values suggests an accuracy of no worse than 50%. The precision, resolution and accuracy of the HCN data are summarized in table 3.11.1.

3.11.6 Data screening

Pressure range: 21–0.1 hPa

Values outside this range are not recommended for scientific use. Data in the 31 hPa to 68 hPa range may prove to be usable after further validation (updates to this document will report any new judgment along those lines).

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Clouds: Clouds have no impact, profiles with non-zero even values of `Status` are suitable for use.

As HCN is only useable in regions unaffected by clouds, profiles which have either, both or neither of the cloud flags set may be used.

Quality: Only profiles whose `Quality` field is greater than 0.2 should be used.

Values of `Quality` are usually near 1.5; occasional lower values do not seem correlated with unusual profiles, but we suggest as a precaution that only profiles with `Quality` > 0.2 be used. Typically this will eliminate only 1–2% of profiles.

Convergence: Only profiles whose `Convergence` field is less than 2.0 should be used.

This should eliminate any chunks which have obviously failed to converge – typically this is only 1–2% of the total.

3.11.7 Artifacts

There are no obvious artifacts within the recommended altitude range

3.11.8 Desired improvements for future data version(s)

Hopefully it will prove possible to make further improvements to the retrieval of HCN in the lower stratosphere.

3.12 Nitric Acid (HNO_3)

Swath name: HNO3

Useful range: 215–1.5 hPa (1.0 hPa under enhanced conditions)

Contact: Michelle Santee, **Email:** <Michelle.L.Santee@jpl.nasa.gov>

3.12.1 Introduction

The standard HNO_3 product is a hybrid constructed by merging retrievals based on radiances from different radiometers: at pressures equal to or greater than 22 hPa, the standard product is derived from the 240-GHz retrievals, whereas above that level (i.e., at lesser pressures), it is derived from the 190-GHz retrievals. The quality and reliability of the Aura MLS v2.2 HNO_3 measurements were assessed in detail by *Santee et al.* [2007]. V3.3*x*/v3.4*x* HNO_3 was greatly improved over that in v2.2; in particular, a low bias through much of the stratosphere (especially evident at pressures greater than or equal to 100 hPa) was largely eliminated. However, the v3.3*x*/v3.4*x* 240-GHz HNO_3 was adversely impacted by clouds [*Livesey et al.*, 2013], leading to a noisy HNO_3 product in the upper troposphere / lower stratosphere (UTLS). The adverse cloud impacts were substantially mitigated in v4.2*x* [*Livesey et al.*, 2020]. For the most part, HNO_3 mixing ratios have not changed dramatically in v5.0*x*. A summary of the estimated precision, resolution (vertical and horizontal), and systematic uncertainty of the v5.0*x* HNO_3 measurements as a function of altitude is given in Table 3.12.1.

3.12.2 Differences between v4.2*x* and v5.0*x*

Figure 3.12.1 shows zonal mean pressure-latitude cross sections of v5.0*x* and v4.2*x* and their differences on selected days for the standard HNO_3 product, which as noted above is composed from the `HNO3-240` and the `HNO3-190` retrievals in the lower and upper parts of the profile, respectively. Figure 3.12.2 shows for the two data versions both the 240-GHz and the 190-GHz retrieved profiles throughout the entire vertical domain, with the "join" level for the hybrid product of 22 hPa marked by the horizontal line. The shapes of mean profiles in the two data versions are very similar throughout the vertical range of the retrievals, and zonal-mean differences are generally small, with a few notable exceptions. First, v5.0*x* abundances are larger at 6.8 hPa, with differences often exceeding 10% in the equatorial and summertime midlatitude regions, as seen in Figure 3.12.1 and the upper right-hand panels in each set of plots in Figure 3.12.2 (compare red and orange curves). Second, at and immediately below the "join" level, tropical mean mixing ratios are typically slightly smaller in v5.0*x*, as seen in the upper left-hand panels in the middle set of plots in Figure 3.12.2 (compare dark and light blue curves at 22 and 46 hPa; not apparent in Figure 3.12.1 as differences are less than 10%). Third, under strongly denitrified conditions at the highest southern latitudes during Antarctic winter, mixing ratios in the stratosphere fluctuate around zero in both versions, leading to alternating large (>30%) positive and negative percent differences (see the July panels in Figure 3.12.1; the disparities between the two versions (dark and light blue curves) are less visible in the July Southern Hemisphere overall polar-cap averages in the bottom-right set of panels in Figure 3.12.2, since these broad averages do not approach zero). Smaller oscillations extend above 10 hPa (Figure 3.12.1), and similar but weaker oscillatory patterns are also present during Arctic winter (though not evident in the figure since the v5.0*x* minus v4.2*x* differences are less than 10%). Finally, mixing ratios in the equatorial region are frequently slightly smaller in v5.0*x* at 100 and/or 147 hPa (Figure 3.12.2, middle set of panels); this change leads to zonal mean values that can be more negative, or negative over a larger area, than those in v4.2*x*, with the small magnitude of the values in this region again resulting in large percent differences (Figure 3.12.1).

Mean profiles computed from measurements taken during the ascending (mainly daytime, solid lines) and descending (mainly nighttime, dashed lines) portions of the orbit are distinguished in Fig-

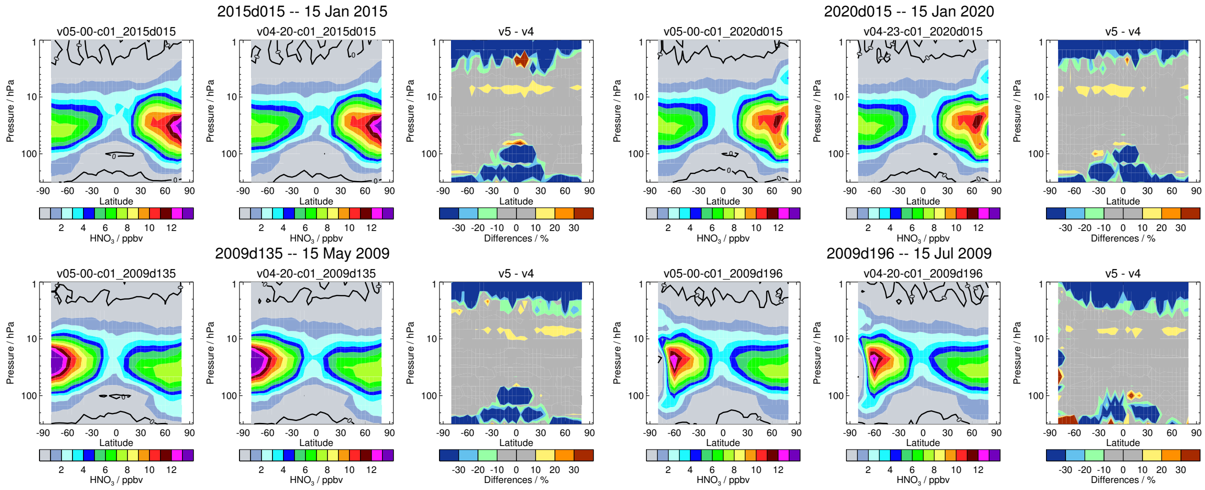

Figure 3.12.1: Zonal mean pressure-latitude cross sections of MLS HNO_3 for four selected days during Arctic (top row) and Antarctic (bottom row) winter under high-HNO_3 (left side) and denitrified (right side) conditions. Each set of plots contains (left) v5.0x, (middle) v4.2x, and (right) their differences (v5.0x minus v4.2x, in percent). The black curves overlaid on the abundance panels (left and middle of each set) mark the zero contour.

ure 3.12.2; as expected, no substantial differences are seen between them in the lower stratosphere or upper troposphere in either version. Figure 3.12.2 also compares the behavior of the two HNO_3 products; in general, the v5.0*x* `HNO3-240` retrieval is slightly smoother at levels above 22 hPa than it was in v4.2*x*, often bringing it somewhat more in line with the `HNO3-190` retrieval, which continues to be used to construct the standard product at those levels.

3.12.3 Resolution

The resolution of the retrieved data can be described using "averaging kernels" [e.g., *Rodgers*, 2000]; the two-dimensional nature of the MLS data processing system means that the kernels describe both vertical and horizontal resolution. Smoothing, imposed on the retrieval system in both the vertical and horizontal directions to enhance retrieval stability and precision, reduces the inherent resolution of the measurements. Thus, although HNO_3 measurements are reported at six pressure levels per decade change in pressure (spacing of ∼2.7 km), the vertical resolution of the v5.0*x* HNO_3 data as determined from the full width at half maximum of the rows of the averaging kernel matrix shown in Figure 3.12.3 varies from ∼3.5 to 5 km over the useful vertical range (see Table 3.12.1 for estimates at individual levels). Substantial overlap in the averaging kernels for the 215 and 316 hPa retrieval surfaces (which both peak at 215 hPa) indicates that the 316 hPa retrieval provides little independent information. Figure 3.12.3 also shows horizontal averaging kernels, from which the along-track horizontal resolution is determined to be ∼350–500 km over most of the vertical range, degrading to 550–800 km at 1.5 and 1 hPa. The cross-track resolution, set by the widths of the fields of view of the 190-GHz and 240-GHz radiometers, is ∼10 km. The along-track separation between adjacent retrieved profiles is 1.5° great circle angle (∼165 km), whereas the longitudinal separation of MLS measurements, set by the Aura orbit, is 10°–20° over low and middle latitudes, with much finer sampling in the polar regions.

3.12.4 Precision

The precision of the MLS HNO_3 measurements is estimated empirically by comparing profiles measured at the intersections of ascending (mainly day) and descending (mainly night) portions of the orbit.

Help Overview Table BrO CH3Cl CH3CN CH3OH ClO CO GPH H2O HCl HCN HNO3 HO2 HOCl IWC IWP N2O O3 OH RHI SO2 T Lvl 3

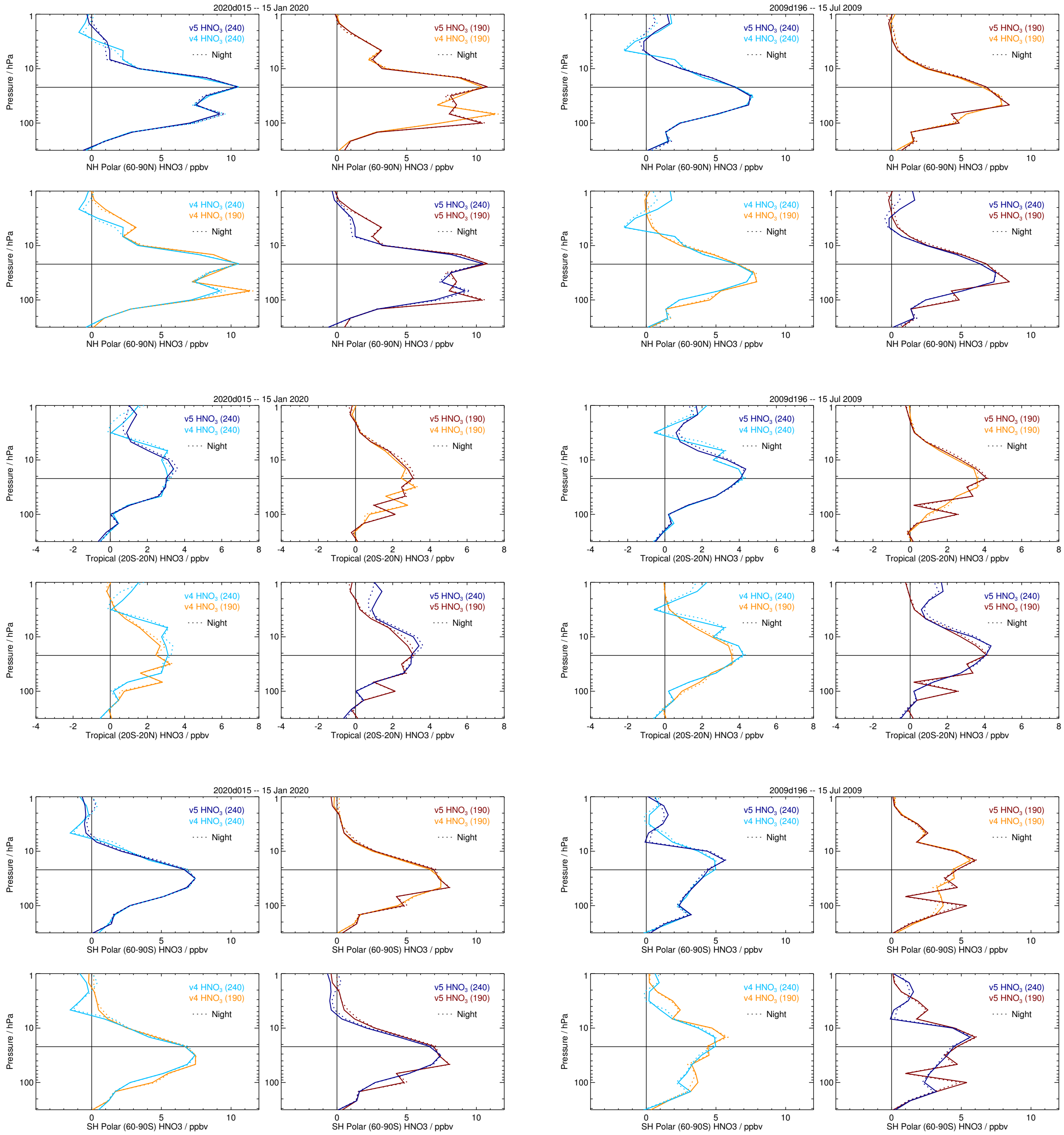

Figure 3.12.2: MLS v5.0x (dark colors) and v4.2x (light colors) profiles of `HNO3-240` (blues) and `HNO3-190` (reds) averaged over the Northern Hemisphere polar (top set), tropical (middle set), and Southern Hemisphere polar (bottom set) regions for a representative day during winter in the Northern (left side) and Southern (right side) Hemispheres. Each set of plots contains four panels, comparing v5.0x and v4.2x `HNO3-240` retrievals, v5.0x and v4.2x `HNO3-190` retrievals, v4.2x `HNO3-240` and `HNO3-190` retrievals, and v5.0x `HNO3-240` and `HNO3-190` retrievals. Solid lines show ascending (mainly daytime) and dashed lines show descending (mainly nighttime) averages. For completeness, full profiles are shown in all panels, but the standard HNO_3 product is derived from the `HNO3-240` retrievals at and at pressures greater than 22 hPa (marked by the horizontal black line) and from the `HNO3-190` retrievals at lower pressures.

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

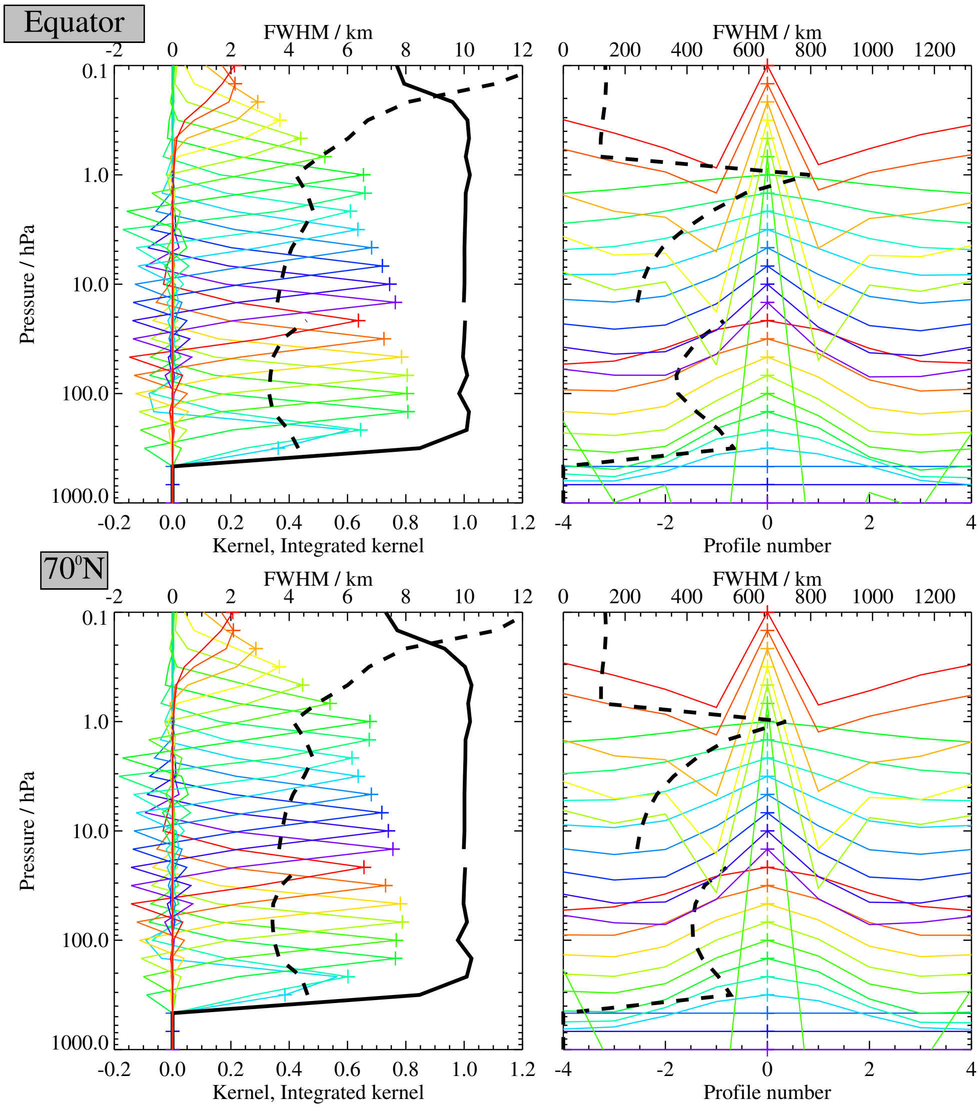

Figure 3.12.3: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x HNO_3 data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

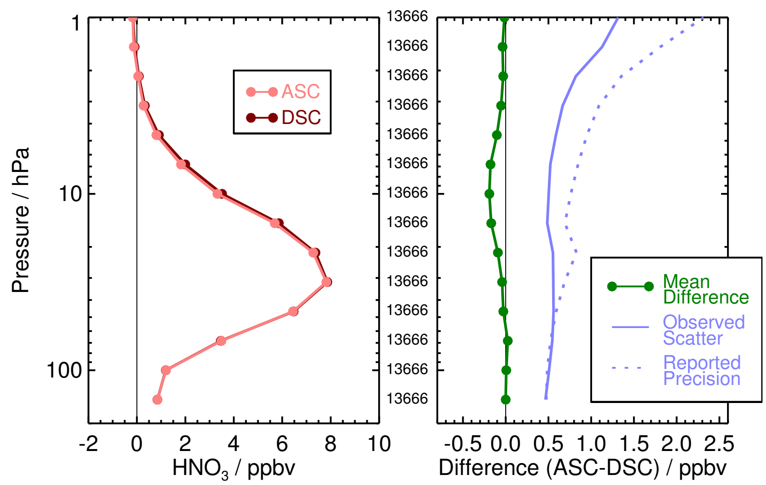

Figure 3.12.4: (left) Ensemble mean profiles for ascending (light red) and descending (dark red) orbit matching pairs of MLS v5.0x HNO_3 profiles averaged over several months of a representative year of data (2009). Symbols indicate MLS retrieval pressure levels. (right) Mean differences (ascending—descending) in pptv (green solid line). Also shown are the standard deviations about the mean differences (light blue solid line) and the root sum square (RSS) of the precisions calculated by the retrieval algorithm for the two sets of profiles (light blue dotted line). The observed scatter about the mean differences and the reported precision values have been scaled by $1/\sqrt{2}$ (to convert from standard deviations of differences into standard deviations of individual data points); hence the light blue solid line represents the statistical repeatability of the MLS measurements, and the light blue dotted line represents the expected 1σ precision for a single profile. The thin black lines mark zero in each panel. The number of crossing pairs of measurements being compared at each pressure level is noted in the space between the panels.

Under ideal conditions (i.e., a quiescent atmosphere), the standard deviation about the mean differences between such matched profile pairs provides a measure of the precision of the individual data points. In practice, however, real changes in the atmosphere may occur over the 12 h interval between the intersecting measurement points, in which case the observed scatter provides an upper limit on the estimate of precision, assuming that the a priori has a negligible influence on the retrieval (a reasonable assumption throughout the retrieval range for HNO_3). The precision estimates were found to be essentially invariant with time; results for several months of a representative year of data are shown in Figure 3.12.4. Mean differences between paired crossing profiles are negligible over most of the profile, indicating the absence of significant systematic ascending / descending biases; small differences in the middle and upper stratosphere may be largely related to photochemical effects. The observed standard deviation values are $\sim$0.6 ppbv or less throughout most of the vertical domain, increasing to $\sim$0.8 ppbv at 2.1 hPa and $\sim$1.2 ppbv above that level. An alternative method of computing the standard deviation of the profiles in the 20°-wide latitude band centered around the equator yields very similar precision estimates.

The observational determination of the precision is compared in Figure 3.12.4 to the theoretical precision values reported by the Level 2 data processing algorithms. Although the two estimates compare very well at the bottom of the recommended vertical range, at pressures smaller than 30 hPa the predicted precision substantially exceeds the observed scatter, indicating that the a priori information and the vertical smoothing (regularization) applied to stabilize the retrieval system and improve the precision are influencing the results at the higher retrieval levels. Because the theoretical precisions take into account occasional variations in instrument performance, the best estimate of the precision of an individual data point is the value quoted for that point in the L2GP files, but it should be borne in mind that this approach overestimates the actual measurement noise at pressures less than 30 hPa.

The single-profile precision estimates cited here are, to first order, independent of latitude and season. However, large geographic variations in HNO_3 abundances give rise to a wide range of signal to noise ratios; thus at some latitudes and altitudes and in some seasons, HNO_3 abundances are smaller than the single-profile precision, necessitating the use of averages for scientific studies. In most cases, precision can be improved by averaging, with the precision of an average of N profiles being $1/\sqrt{N}$ times the precision of an individual profile (note that this is not the case for averages of successive along-track profiles, which are not completely independent because of horizontal smearing).

3.12.5 Accuracy

The effects of various sources of systematic uncertainty (e.g., instrumental issues, spectroscopic uncertainty, and approximations in the retrieval formulation and implementation) on the MLS v5.0*x* HNO_3 measurements have been quantified through a comprehensive set of retrievals of synthetic radiances; see *Santee et al.* [2007] for details of a similar analysis conducted on MLS v2.2 HNO_3 data. The overall systematic uncertainty, or accuracy, is calculated by combining (RSS) the contributions from both the expected biases and the additional scatter each source of uncertainty may introduce into the data. In aggregate, the factors considered in these simulations are estimated to give rise to a total systematic uncertainty ranging from approximately 0.1 to 2.2 ppbv, depending on the level, in the MLS v5.0*x* HNO_3 data (see Table 3.12.1).

3.12.6 Comparisons with other datasets

Extensive comparisons of MLS v2.2 HNO_3 data with a variety of different platforms (ground-based, balloon-borne, aircraft, and satellite instruments) were presented by *Santee et al.* [2007]. Comparisons of v5.0*x* HNO_3 with correlative data have not been conducted but are expected to yield results similar to those for previous versions.

3.12.7 Data screening – all data

Pressure range: 215–1.5 hPa

Values outside this range are not recommended for scientific use. The HNO_3 data at 1.0 hPa and lower pressures may be useful under certain enhanced conditions but should not be analyzed in scientific studies without significant discussion with the MLS science team.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

3.12.8 Data screening – upper troposphere / lower stratosphere (pressures of 22 hPa or greater)

The `Quality` and `Convergence` fields included in the `HNO3` swath in the standard `L2GP-HNO3` files are appropriate for use in screening the data at and below (i.e., at pressures greater than) 22 hPa. For those levels:

Quality: Only profiles whose `Quality` field is greater than 0.8 should be used.

This threshold for `Quality` (unchanged from v4.2*x*) is a fairly conservative value that typically excludes a substantial fraction (∼1–3%) of HNO_3 profiles on a daily basis, potentially discarding "good" data points while not necessarily identifying all "bad" ones. As in previous versions, many HNO_3 profiles in v5.0*x* are characterized by a "notch", with unexpectedly low (often negative in the tropics) values at 100 or 147 hPa and higher values at the level below; although a number of such oscillatory profiles are removed through filtering using the `Quality` field, in many cases mean profiles continue to display a prominent notch.

Convergence: Only profiles whose `Convergence` field is less than 1.03 should be used.

On a typical day this threshold for `Convergence` (unchanged from v4.2*x*) discards few (0.5% or less) of the HNO_3 profiles, some of which show unphysical behavior.

Status flag: Only use profiles for which the `Status` field is zero.

Nonzero but even values of `Status` indicate that the profile has been marked as questionable, typically because the measurements may have been affected by the presence of thick clouds. In the lowermost stratosphere and upper troposphere, thick clouds can lead to spikes in the HNO_3 mixing ratios in the equatorial regions. Therefore, it is recommended that at and below (i.e., at pressures greater than) 68 hPa all profiles with nonzero values of `Status` be discarded because of the potential for cloud contamination. Globally ∼1–2% of profiles are identified in this manner, with the fraction of profiles possibly impacted by clouds rising to ∼5% on average in the tropics. While this procedure will reject some profiles that are probably not significantly impacted by cloud effects, and the number of profiles rejected that are not flagged by other criteria is small (∼0.5 to 1% of total profiles), it does eliminate some unphysical profiles that are not filtered by other means. See Section 1.6 for more information on the interpretation of the `Status` field.

3.12.9 Data screening – upper stratosphere (pressures of 15 hPa or less)

The above screening criteria *should not be used* for data at 15 hPa and higher altitudes (lower pressures). Rather, the appropriate indicators to be used in masking HNO_3 data at these altitudes are the `Quality` and `Convergence` values pertinent to the 190-GHz retrievals. To aid that screening, the `HNO3-190` swath has been included in the standard HNO_3 files for v5.0*x*. The following screening criteria are based on the 190-GHz HNO_3 information:

Quality: Only profiles with a value of the `Quality` field for `HNO3-190` greater than 0.8 should be used.

This threshold for `Quality` (unchanged from v4.2*x*) typically excludes ∼1–3% of HNO_3 profiles on a daily basis; it is a conservative value that potentially discards some “good” data points while not necessarily identifying all “bad” ones.

Convergence: Only profiles with a value of the `Convergence` field for the `HNO3-190` product less than 1.4 should be used.

On a typical day this threshold for `Convergence` discards ∼0.5–2% of the HNO_3 profiles. Many of the profiles thus flagged show some unphysical behavior, especially at the highest altitudes in the recommended range.

Status flag: Only use profiles for which the `Status` field is an even number.

Clouds generally have little influence on the stratospheric HNO_3 data at these altitudes, thus profiles for which the `HNO3-190 Status` field is a nonzero even number can be used without restriction.

3.12.10 Artifacts

A persistent “notch” in the profile, with low values at 100 or 147 hPa and higher values at the level below, is most pronounced in the tropics (Figure 3.12.2) and midlatitudes but is also apparent at high latitudes in some seasons. The origin of this oscillatory signature in the retrievals is unclear; it is reduced but by no means eliminated through application of the recommended screening procedures. Users of the MLS HNO_3 data are cautioned that retrieved abundances can be strongly negative in the tropical UTLS, even for mean profiles, and are advised to consult with the MLS science team before undertaking scientific studies of that region relying on the v5.0*x* HNO_3 data.

3.12.11 Desired improvements for future data version(s)

Further work to diagnose and eliminate the persistent unphysical oscillations at the lowest retrieval levels will be explored in future.

Table 3.12.1: Summary of Aura MLS v5.0x HNO_3 Characteristics

Pressure / hPa	Resolution V × H[a] / km	Precision[b] / ppbv	Systematic Uncertainty[c] / ppbv	Comments
0.68–0.001	—	—	—	Unsuitable for scientific use
1.5–1.0	4–4.5 × 550–800	±1.2	±0.3	Caution, averaging recommended
2.1	5 × 450–500	±0.8	±0.5	
3.2	4.5 × 350–400	±0.6	±0.1	
15–4.6	3.5–4 × 250–350	±0.6	±0.5–0.7	
22	4.5 × 500	±0.6	±2.2	
32	4 × 450	±0.6	±1.4	
147–46	3.5 × 400–450	±0.6	±1.0	Consult MLS team for use in tropical UTLS
215	4.5 × 500	±0.6	±1.1	Consult MLS team for use in tropical UTLS
316	—	—	—	Unsuitable for scientific use
1000–464	—	—	—	Not retrieved

[a]Horizontal resolution in along-track direction.
[b]Precision on individual profiles, determined from observed scatter in the data in a region of minimal atmospheric variability.
[c]Values should be interpreted as 2-σ estimates of the probable magnitude.

3.13 Peroxy Radical (HO_2)

Swath name: HO2

Useful range: 22–0.046 hPa

Contact: Luis Millán, **Email:** <Luis.F.Millan@jpl.nasa.gov>

3.13.1 Introduction

A description of HO_2 data quality, precision, systematic errors, and validation for an earlier version, v2.2, is given in *Pickett et al.* [2006b]. An early validation using v1.5 software is also described in *Pickett et al.* [2006b]. The estimated uncertainties, precisions, and resolution for v5.0*x* HO_2 are summarized below in Table 3.13.1.

An algorithm to retrieve daily zonal means of HO_2 over an extended vertical range by first averaging the radiances has been developed by the MLS team [*Millán et al.*, 2015]. This alternative dataset is the first long-term daytime and nighttime HO_2 satellite record covering the stratosphere and the mesosphere. This dataset is available from the GSFC DISC. The product short name is "ML3DZMHO2".

3.13.2 Resolution

Figure 3.13.1 shows the HO_2 averaging kernel for daytime at 70°N and the Equator. The latitudinal variation in the averaging kernel is very small. The vertical resolution for pressures greater than 0.1 hPa is generally about 5 km.

3.13.3 Precision

A typical HO_2 profile and the associated precisions (for both v4.2*x* and v5.0*x*) are shown in Figure 3.13.2. The profile is shown in both volume mixing ratio (vmr) and density units. All MLS data are reported in vmr for consistency with the other retrieved molecules. However, use of density units (10^6 cm^{-3}) reduces the apparent steep gradient of HO_2 vertical profile, allowing one to see the profile with more detail. The night HO_2 profile is expected to exhibit a narrow layer near the altitudes of the nighttime OH layer at ~82 km [*Pickett et al.*, 2006a], which is not shown in Figure 3.13.2 since MLS HO_2 data is not recommended for altitudes above 0.046 hPa (~70 km). Precisions are such that an HO_2 zonal average within a 10° latitude bin can be determined with better than 10% relative precision with 20 days of data (~2000 samples) for most pressure levels over 22–0.046 hPa.

3.13.4 Accuracy

Table 3.13.1 summarizes the accuracy expected for HO_2. The effect of each identified source of systematic error on MLS measurements of radiance has been quantified and modeled [*Read et al.*, 2007]. These quantified effects correspond to either 2σ estimates of uncertainties in each MLS product, or an estimate of the maximum reasonable uncertainty based on instrument knowledge and/or design requirements. The HO_2 bias can be eliminated by taking day-night differences over the entire recommended pressure range. The overall uncertainty is the square root of the sum of squares of the precision and accuracy.

3.13.5 Data screening

It is recommended that HO_2 data values be used in scientific investigations if all the following tests are successful:

Pressure range: 22–0.046 hPa

Values outside this range are not recommended for scientific use.

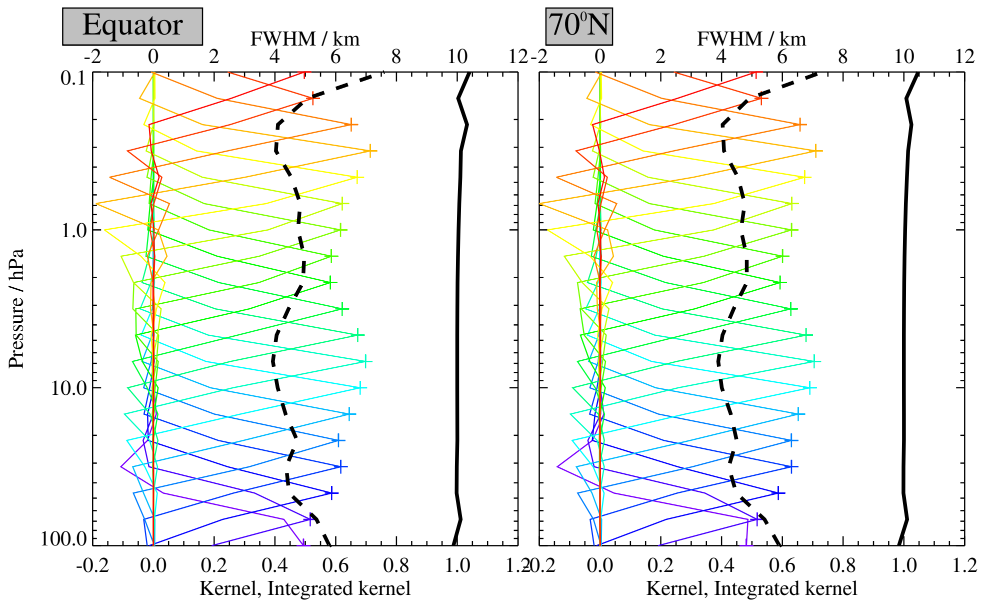

Figure 3.13.1: Typical vertical averaging kernels for the MLS v5.0x HO_2 data at the equator (left) and at 70°N (right); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the vertical resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). The solid black line shows the integrated area under each kernel; values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. The low signal to noise for this product necessitates the use of significant averaging (e.g., monthly zonal mean), making horizontal averaging kernels largely irrelevant.

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

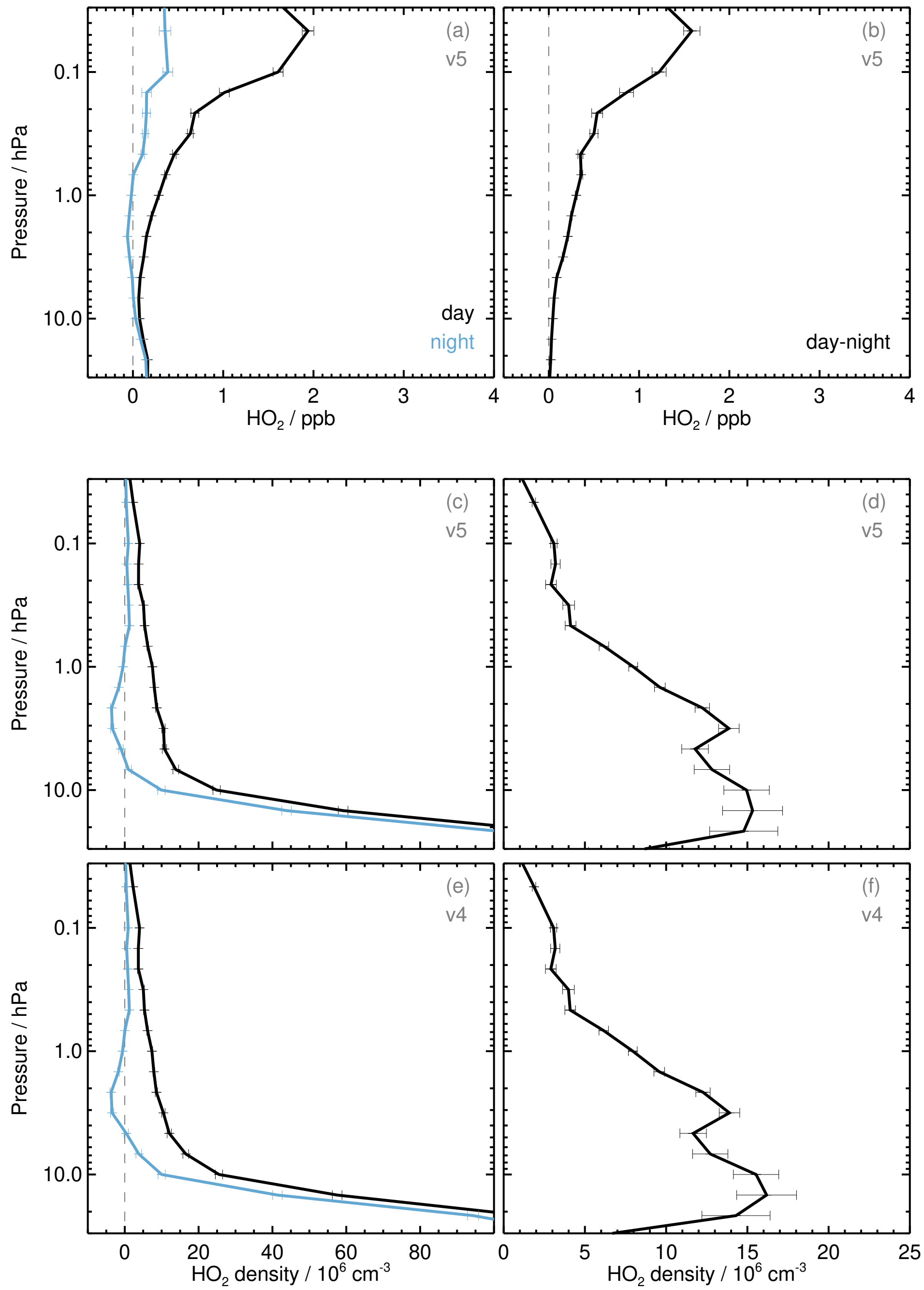

Figure 3.13.2: Monthly zonal mean of retrieved HO_2 and its estimated precision (horizontal error bars) for January, 2009 averaged over 29°N to 39°N. Panel (a) shows v5.0x HO_2 vmr vs. pressure for day (black) and night (blue). Panel (b) shows the same data plotted as a day-night difference (note that a day-night difference is required for HO_2 for all pressure levels). Panel (c) shows the same data in (a) converted into density units. Panel (d) shows the day-night differences for the data in panel (c). Panels (e) and (f) are equivalent to (c) and (d) but using v4.2x data.

Table 3.13.1: Summary of precisions, resolution, and uncertainties for the MLS v5.0x HO_2 product

Pressure / hPa	Vertical resolution km	Precision[a] / 10^6 cm^{-3}	Day–night accuracy / 10^6 cm^{-3}	Comments
$<$ 0.03 hPa	—	—	—	Unsuitable for scientific use
0.046 hPa	10	4	0.01	Use day–night difference
0.10 hPa	7	8	0.2	Use day–night difference
1.0 hPa	5	11	0.2	Use day–night difference
10 hPa	4	56	11	Use day–night difference
$>$ 22 hPa	—	—	—	Unsuitable for scientific use

[a]Precision for a single profile

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality: MLS v5.0*x* HO_2 data can be used irrespective of the value of the `Quality` field.

Convergence: Only profiles whose `Convergence` field is less than 1.1 should be used.

In version v2.2 this test often fails for 100 out of 3500 profiles in a day. In the current version, v5.0*x*, there are often zero or very few non-converged profiles.

3.13.6 Artifacts

Currently there are no known artifacts in the HO_2 product. The primary limitation is the precision and the altitude range.

3.13.7 Review of comparisons with other datasets

HO_2 data from MLS v2.2 software have been validated with two balloon-borne remote-sensing instruments. Details of the comparison are given in *Pickett et al.* [2006b]. Differences between v2.2 and v5.0*x* show no differences large enough to alter results of previous validation studies.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

3.14 Hypochlorous Acid (HOCl)

Swath name: `HOCl`

Useful range: 10–2.2 hPa

Contact: Lucien Froidevaux, **Email:** <Lucien.Froidevaux@jpl.nasa.gov>

3.14.1 Introduction

There has been little change in the v5.0*x* HOCl retrievals, and small changes are well within the somewhat large estimated accuracies (systematic uncertainties). We provide below sample mean HOCl distributions for the v5.0*x* and v4.2*x* data versions, and their differences. Otherwise, previous information regarding this species remains largely unchanged; the main points are mentioned here mainly for new data users.

The HOCl retrieval is quite noisy for individual profiles and HOCl data require some averaging (e.g., in 10° zonal means for one or more weeks) to get useful precision of better than 10 pptv, in comparison to typical upper stratospheric HOCl abundances of 100–150 pptv. Table 3.14.1 summarizes the MLS HOCl resolution, precision, and accuracy estimates for the upper stratosphere. More discussion and a brief validation summary are given in the following sections, along with data screening recommendations.

An algorithm to retrieve daily zonal means of HOCl by first averaging the radiances has been developed by the MLS team [*Froidevaux et al.*, 2021], building on the work described in *Millán et al.* [2012] and *Millán et al.* [2015] for BrO and HO_2, respectively. This dataset reduces slightly the variability and will be available from the GSFC DISC soon.

3.14.2 Changes from v4.2*x*

There were no large algorithmic changes relating directly to HOCl for the v5.0*x* retrievals. However, given the small level of HOCl spectral radiance signal, the retrieved HOCl abundances can be sensitive, indirectly, to even minor changes in the retrieval system. The (small) changes that seem to have contributed to the HOCl differences for v5.0*x* include some changes to nitric acid in the R4 (640 GHz) retrievals, in conjunction with (or tied to) changes from other bands (e.g., via differences in tangent pressure, temperature, and water vapor), and changes to the a priori values for certain species (nitric acid, ozone, and water vapor).

The background observed in the 640-GHz radiances includes emissions from N_2, O_2, and H_2O. There are laboratory-based and ground-based models for the continuum absorptions that are the basis for the MLS absorption model [*Pardo et al.*, 2001, and references therein]. These models were tested against MLS extinction measurements from the wing channels in the 640-GHz radiometer. The latitude dependence of this extinction was found to agree better with the expected moist plus dry continuum extinction values if the dry and moist continuum functions were scaled by factors close to 20%; however, this aspect is no different than what was done in the previous data version.

A comparison plot showing zonal average upper stratospheric HOCl contours (from 10 to 2 hPa) and differences between the two data versions for a typical month (March, 2009) is provided in Figure 3.14.1. The average v5.0*x* HOCl abundances are slightly smaller than the v4.2*x* retrievals, typically by about 10 pptv (or 10%), with slightly larger values than in v4.2*x* from 2 to 1 hPa. The estimated precision values are essentially unchanged from v4.2*x*.

3.14.3 Resolution

Based on the width of the averaging kernels shown in Figure 3.14.2, the vertical resolution for upper stratospheric HOCl is ~6 km (significantly worse than the 640-GHz radiometer vertical field of view width of 1.4 km). This reflects the choice of smoothing constraints for HOCl which favor precision over vertical resolution.

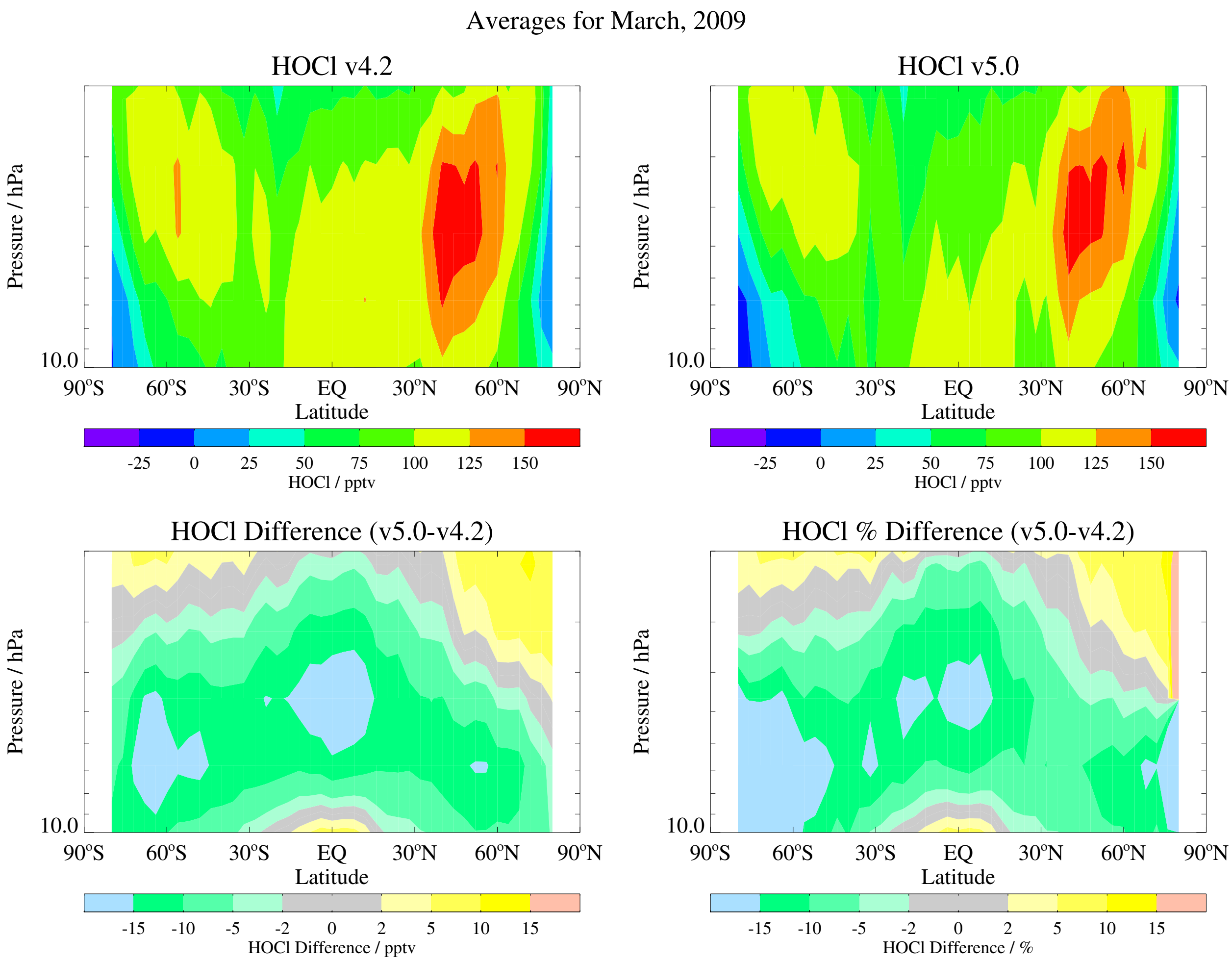

Figure 3.14.1: Zonal averages for upper stratospheric MLS HOCl profiles during March, 2009, showing the MLS v4.2x HOCl mixing ratio contours (top left panel), the v5.0x contours (top right panel), and their differences in pptv (v5.0x minus v4.2x, bottom left panel) and percent (v5.0x minus v4.2x versus v4.2x, bottom right panel).

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

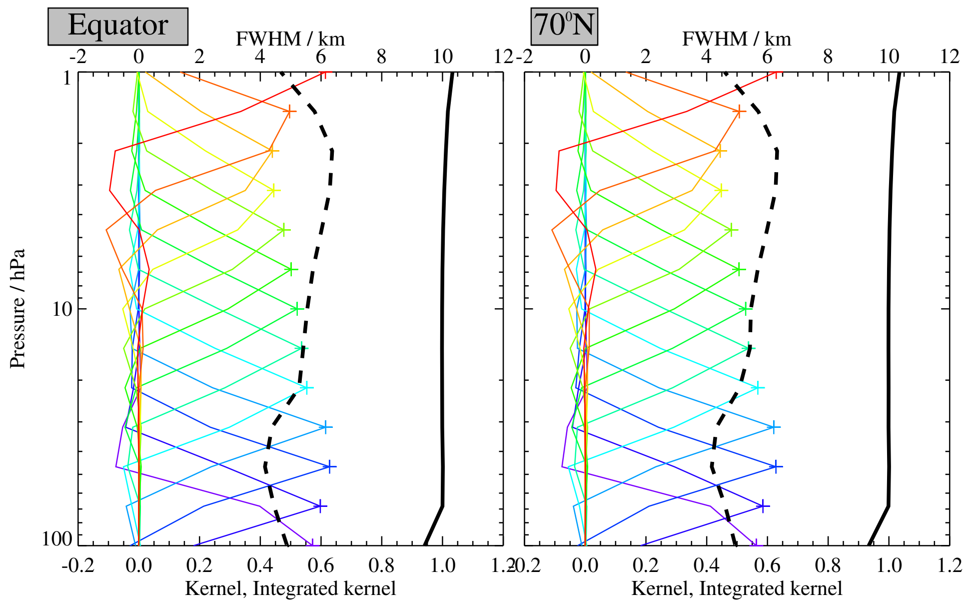

Figure 3.14.2: Typical vertical averaging kernels for the MLS v5.0x HOCl data at the equator (left) and at 70°N (right); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the vertical resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). The solid black line shows the integrated area under each kernel; values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. The low signal to noise for this product necessitates the use of significant averaging (e.g., monthly zonal mean), making horizontal averaging kernels largely irrelevant.

3.14.4 Precision

The estimated single-profile precision reported by the Level 2 software is about 300 to 400 pptv in the upper stratosphere. A more useful number of 10 pptv is quoted in Table 3.14.1 for the typical precision of a 10° weekly zonal means for this product.

3.14.5 Accuracy

The accuracy estimates shown in Table 3.14.1 come from a formal quantification of the combined effects of possible systematic errors in MLS calibration, spectroscopy, etc. on the HOCl retrievals [*Read et al.*, 2007]. These values are intended to represent 2σ estimates of accuracy. The largest contributors to possible errors for HOCl are contaminant species, gain compression, and sideband ratio uncertainties. The Table gives a range of error estimates. The average changes for upper stratospheric HOCl between v4.2*x* and v5.0*x* are well within the quoted accuracy estimates (which may be somewhat conservative). The HOCl signal becomes too small compared to the systematic uncertainties to allow for reliable retrievals at pressures larger than 10 hPa.

3.14.6 Data screening

Pressure range: 10–2.2 hPa

Values outside this range are not recommended for scientific use. Artifacts (negative averages) for pressures larger than about 10 hPa make this product unsuitable for use in the lower stratosphere. Regarding the topmost altitude range, the sensitivity to *a priori* increases rapidly at pressures of 1 hPa or less; we continue to recommend the use of (average) HOCl values only up to 2.2 hPa.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality field: Only profiles with a value of the `Quality` field *greater* than 1.2 should be used.

This criterion removes profiles with the poorest radiance fits, typically less than 0.1% of the daily profiles. For HOCl, this screening correlates well with the poorly converged sets of profiles (see below); we recommend the use of both the `Quality` and `Convergence` fields for data screening.

Convergence field: Only profiles with a value of the `Convergence` field *less* than 1.05 should be used.

For the vast majority of profiles (99% or more for most days), this field is less than 1.05. Nevertheless, on occasion, sets of profiles (typically one or more groups of ten profiles, retrieved as a 'chunk') have this `Convergence` field set to larger values, and should be discarded.

Clouds: Profiles identified as being affected by clouds can be used with no restriction.

3.14.7 Review of comparisons with other datasets

The MLS HOCl retrievals exhibit the expected morphology in monthly mean latitude / pressure contour plots; for example, such plots for September months from MLS compare favorably, to first-order, with results produced by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) for September, 2002 [*von Clarmann et al.*, 2006]. MLS HOCl averages at midlatitudes are close to the results from balloon-borne infrared measurements. Generally favorable comparisons (within the error bars) have been made of the diurnal changes in upper stratospheric HOCl between Aura MLS (v3.3), other satellite datasets, and a 1-D photochemical model [*Khosravi et al.*, 2013].

Table 3.14.1: Summary for MLS hypochlorous acid

Pressure	Precision[a]		Vertical Resolution	Accuracy[b]		Comments
hPa	pptv	%	km	pptv	%	
1.5 or less	—	—	—	—	—	Unsuitable for scientific use
2.2 to 10	5–10	5–20	5.5–6	40–80	25–100	Some averaging required
15 or more	—	—	—	—	—	Unsuitable for scientific use

[a]Precision (1σ) for 1 week/10 degrees zonal means or 2 weeks/5 degrees zonal means
[b]2σ estimate from systematic uncertainty characterization tests

3.14.8 Artifacts

- The 640-GHz radiometer bands 10 (for ClO) and 29 (for HOCl) were turned off for a few time periods in 2006 to investigate degradation issues that might affect these channels in the future. These bands were off on April 8,9, and 10, 2006, and also for April 17, 2006 (after 19:52 UT) through May 17, 2006. There are essentially no useful HOCl (or ClO) data for these time periods. The v5.0*x* (as for previous data versions) software correctly flags these incidents with poor (odd) `Status` values (which should be screened out).
- There are significant artifacts in the mean values (large negative values) for HOCl in the lower stratosphere, where the use of this product is not recommended.
- Users should screen out the non-converged and poorest quality HOCl profiles, as such profiles (typically a very small number per day) tend to behave unlike the majority of the other MLS retrievals. See the criteria listed above.

Help Overview Table BrO CH3Cl CH3CN CH3OH ClO CO GPH H2O HCl HCN HNO3 HO2 HOCl IWC IWP N2O O3 OH RHI SO2 T Lvl 3

3.15 Cloud Ice Water Content (IWC)

Swath name: `IWC`

Units: g/m^3

Useful range: 215–83 hPa

Contact: Alyn Lambert, **Email:** <Alyn.Lambert@jpl.nasa.gov>

3.15.1 Introduction

The MLS IWC is retrieved from cloud-induced radiances (T_{cir}) of the 240-GHz window channel in a separate processing step after the atmospheric state (Temperature and tangent height pressure) and important gaseous species (H_2O, O_3, HNO_3) have been finalized in the retrieval processing. The derived T_{cir} are binned onto the standard horizontal (1.5° along track) and vertical (12 surfaces per decade change in pressure) grids, and converted to IWC using the modeled T_{cir}–IWC relations [*Wu et al.*, 2006]. The standard IWC profile has a useful vertical range between 215–83 hPa although the validation has been conducted for a subset of the range of IWC values. IWC measurements beyond the value ranges specified in Table 3.15.1 are to be regarded currently as giving only qualitative information on cloud ice. They require further validation for quantitative interpretation.

3.15.2 Resolution

In the IWC ranges specified in Table 3.15.1, each MLS measurement can be quantitatively interpreted as the average IWC for the volume sampled. This volume has a vertical extent of ∼3 km, with ∼300 km and 7 km along and cross track respectively.

3.15.3 Precision

The precision values quoted in the IWC files do not represent the true precision of the data. The precision for a particular measurement must be evaluated on a daily basis using the method described in the screening section below. The precision listed in Table 3.15.1 reflects typical values obtained from the method described below.

3.15.4 Accuracy

The IWC accuracy values listed in Table 3.15.1 are estimates from comparisons of the earlier v2.2 MLS data product with CloudSat and detailed analyses on the v2.2 error budget can be found in *Wu et al.* [2008].

3.15.5 Data screening

Pressure range (215–83 hPa): Values outside this range are not recommended for scientific use. The maximum detectable IWC is ∼100 mg/m^3.

Use Temperature Status, Quality and Convergence: The user is recommended to screen the IWC data using the `Status` field in the collocated temperature profile to exclude bad retrievals [*Schwartz et al.*, 2008]. In other words, only IWC profiles for which temperature `Status` is an even number should be used. Similarly, the users should only use IWC profiles where the corresponding Temperature profiles have *Quality* of 0.9 or larger and `Convergence` less than 1.03.

Other screening: The IWC product derives from differences between measured radiances and those predicted assuming cloud free conditions. Spectroscopic and calibration uncertainties give rise to temporally and geographically varying biases in this difference, and hence the IWC product. These biases must be iteratively identified and removed, using a "2σ, 3σ" screening method, as described below.

1. Uncertainties in spectroscopy and atmospheric composition are manifested as residual biases in the IWC fields which should be identified and removed as follows. IWC data should be averaged in a 10° latitude bins and outliers rejected iteratively by excluding measurements greater than 2σ standard deviation about the mean (μ) of the bin. Repeat the σ and μ calculations after every new set of rejections. Convergence is usually reached within 5–10 iterations, and the final σ is the estimated precision for the IWC measurements.
2. Interpolate the final σ and μ to the latitude of each measurement, and subtract μ from IWC for each measurement.
3. Finally, apply the 3σ threshold to determine if an IWC measurement is statistically significant. In other words, it must have IWC $> \mu + 3\sigma$ in order to be considered as a significant cloud hit. The 3σ threshold is needed for cloud detection since a small percentage of clear-sky residual noise can result in a large percentage of "false alarms" in cloud detection.

3.15.6 Artifacts

At wintertime mid-to-high latitudes, strong stratospheric gravity waves may induce large fluctuations in the retrieved tangent pressure, and cause false cloud detection with the "2σ, 3σ" screening method. The false cloud detection seems to affect the 100 hPa pressure level most, as expected for such impact coming from the lower stratosphere.

3.15.7 Comparisons with other datasets

Scatter plots of v5.0*x* vs v2.2 IWC show mean biases of less than 10% in the pressure range 215–83 hPa and histograms show that the random noise in v5.0*x* IWC is generally larger than in v2.2 (see Figure 3.15.1 and Table 3.15.1). However, in localized regions, there can be substantial differences in IWC values between these versions that are driven by the reaction of the IWC retrieval to the changes in v5.0*x* UTLS H_2O. These effects are largest at pressures of 215 hPa and higher and have been verified by examining the negative correlations between the changes in H_2O and IWC.

Apart from the differences noted above, the MLS v5.0*x* IWC is similar to the MLS v2.2 product described and validated in *Wu et al.* [2008]. A revised validation paper for IWC is not planned in the near future and users are encouraged to read *Wu et al.* [2008] for more information.

Comparisons between v2.2 MLS and CloudSat IWC showed good agreement with PDF differences <50% for the IWC ranges specified in Table 3.15.1. Comparisons with AIRS, OMI and MODIS suggest that MLS cloud tops are slightly higher by ~1 km than the correlative data in general.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

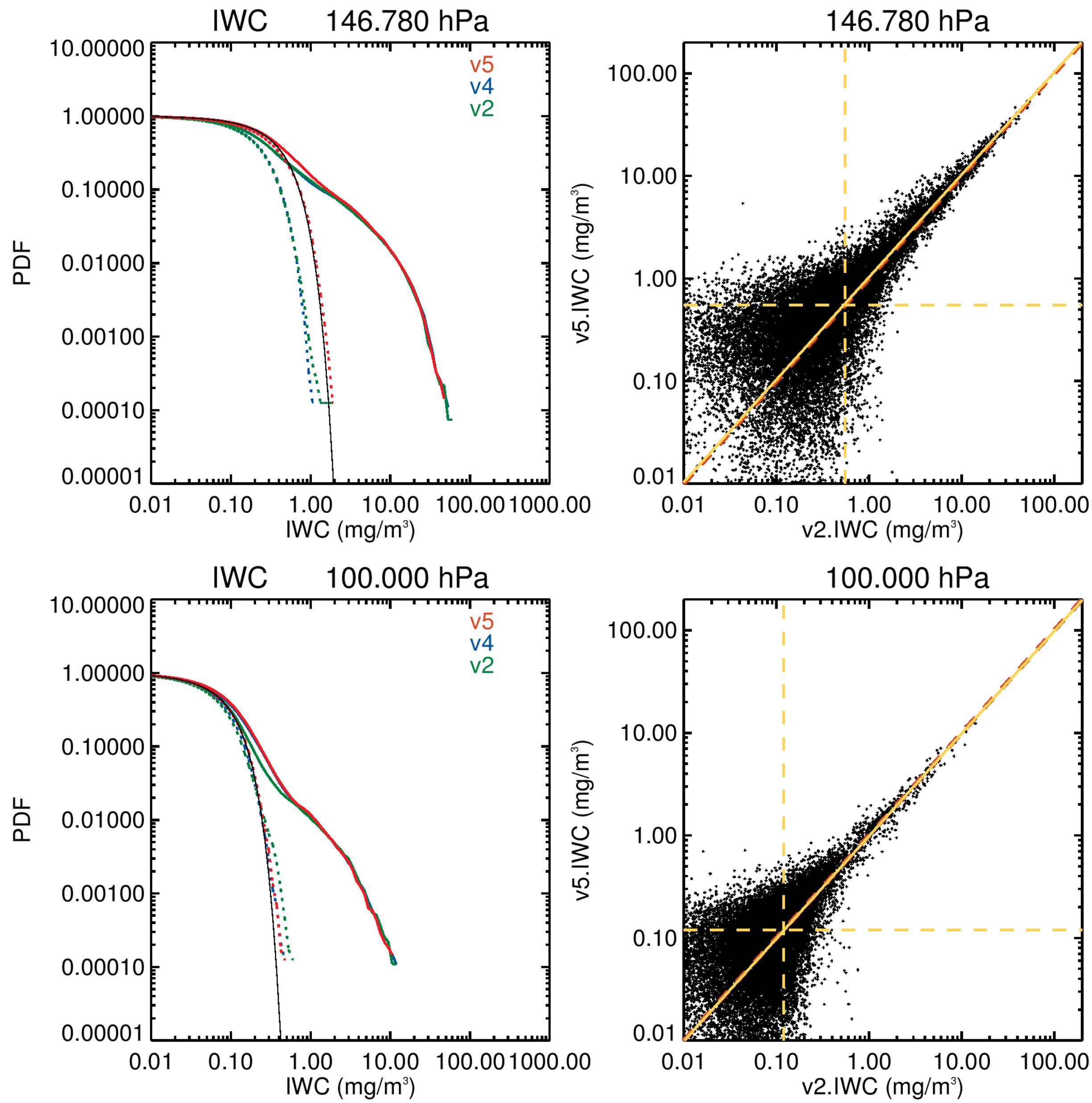

Figure 3.15.1: MLS v5, v4 and v2 IWC comparisons for July 2009 at 146 hPa and 100 hPa. (a) Left: Probability density functions (PDF) (v5, red; v4, blue; and v2, green) with dashed lines showing the corresponding noise levels (obtained by folding the negative IWC values about the origin) and the thin black lines representing the Gaussian error function. (b) Right: Scatter plots of IWC v5 vs. v2 (black points) with dashed red lines indicating the 1:1 line, dashed yellow lines the 1σ uncertainties. The solid yellow lines are linear fits to the data (which lie practically on the 1:1 line).

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

Table 3.15.1: Summary of MLS v5.0x IWC precision, accuracy, and resolution.

Pressure / hPa	Resolution[a] / km	Typical precision[b] / mg/m^3	Accuracy[c] / mg/m^3		Valid IWC range[d] / mg/m^3
			$<10\,mg/m^3$	$>10\,mg/m^3$	
p<70	Unsuitable for scientific use				
83	200×7×5	0.06–0.15	100%	—	0.02–50
100	200×7×5	0.08–0.18	100%	150%	0.02–50
121	250×7×4	0.08–0.24	100%	100%	0.04–50
147	300×7×4	0.20–0.65	100%	100%	0.1–50
177	300×7×4	0.5–2.3	150%	100%	0.3–50
215	300×7×4	1.2–5.5	300%	100%	0.6–50
p>260	Unsuitable for scientific use				

[a] The along-track, cross-track and vertical extent, respectively of the atmospheric volume sampled by an individual MLS measurement.

[b] These are typical 1σ precisions where the better values are for the extratropics and the poorer values for the tropics. The precision for a particular measurement must be evaluated on a daily basis using the method described in the text.

[c] Estimated from comparisons with CloudSat.

[d] This is the range where the stated precision, accuracy and resolution are applied. In this range MLS measurements can be quantitatively interpreted as the average IWC for the volume sampled. IWC values above this range, currently giving qualitative information on cloud ice, require further validation for quantitative interpretation.

3.16 Cloud Ice Water Path (IWP)

Swath name: IWP (stored as an additional swath in the L2GP-IWC file).

Units: g/m^2

Useful range: MLS IWP is the ice water column above ~6 km

Contact: Alyn Lambert, **Email:** <Alyn.Lambert@jpl.nasa.gov>

3.16.1 Introduction

MLS standard IWP is retrieved from cloud-induced radiances (T_{cir}) of the 240-GHz window channel at 650 hPa tangent pressure (see Figure 3.16.1). It represents a partial column above ∼6 km, and is stored in the v5.0*x* L2GP IWC file as a separate swath. For the IWP retrieval, T_{cir} is first converted to a near horizontal slant path (with a ∼3° elevation angle) IWP "hIWP", using the modeled T_{cir}–hIWP relation. The hIWP is then converted to the nadir IWP at the tangent point location, and interpolated to the MLS standard horizontal grid.

3.16.2 Resolution

In the IWP ranges specified in the summary at the end of this section, each MLS measurement can be quantitatively interpreted as the average IWP for the volume sampled. The MLS IWP volume is a vertical column above ∼6 km, with 60 km and 7 km along and cross track extent, respectively.

3.16.3 Precision

The precision values quoted in the IWP swaths do not represent the true precision of the data. The precision for a particular measurement must be evaluated on a daily basis using the method described in the screening section below. The 3 g/m^2 precision given the summary at the end of this section reflects *typical values* for MLS IWP measurements.

3.16.4 Accuracy

The IWP accuracy is ∼50%, as estimated from comparisons of the earlier v2.2 MLS data product with CloudSat and detailed analyses on the v2.2 error budget can be found in *Wu et al.* [2009].

3.16.5 Data screening

Sensitivity: The standard IWP product has a useful sensitivity up to 200 g/m^2 where MLS measurements can be quantitatively interpreted as the average IWP for the volume sampled.

Use Temperature Status, Quality and Convergence: The user is recommended to screen the IWP data using the `Status` field in the collocated temperature profile to exclude bad retrievals [*Schwartz et al.*, 2008]. In other words, only IWP values for which temperature `Status` is an even number should be used. Similarly, the users should only use IWP values where the corresponding Temperature profiles have *Quality* of 0.9 or larger and `Convergence` less than 1.03.

Other screening: the user is also recommended to screen the IWP data for significant cloud hits on a daily basis using the "2σ, 3σ" method described in the IWC section (3.15). The 3σ threshold is needed for cloud detection since a small percentage of clear-sky residual noise can result in a large percentage of false alarm in cloud detection.

3.16.6 Artifacts

High-latitude high-land surface can be mistakenly detected as a cloud when the atmosphere is very dry, allowing MLS 240-GHz radiances to penetrate down to the surface. Surface emission/scattering can then reduce brightness temperature. Surface effects (e.g., over the highland over Antarctica) may introduce artificial IWP values as large as 10 g/m^2. In addition, the geographical location of MLS IWP is currently registered at the tangent point, which is ∼2 profiles away from the actual location of the IWP column as shown in Figure 3.16.1. The user needs to correct this offset by replacing the IWP location with the one at 2 profiles earlier.

3.16.7 Comparisons with other datasets

Compared to v2.2 IWP the v5.0*x* IWP values are systematically smaller by ∼4 % and the random noise is slightly smaller than in v2.2 (see Figure 3.16.2). Apart from the differences noted above, the MLS v5.0*x* IWP is similar to the MLS v2.2 product described and validated in *Wu et al.* [2009]. A revised validation paper for IWP is not planned in the near future and users are advised to read *Wu et al.* [2009] for more information.

Comparisons between v2.2 MLS and CloudSat IWP showed good agreement with PDF differences <50% for the IWP range specified in the summary at the end of this section.

3.16.8 Desired improvements for future data version(s)

The IWP retrieval in v5.0*x* is a simple first-order conversion, applied independently to each T_{cir} measurement. Plans for future versions include development of 2-D cloudy-sky radiative transfer model. This will allow IWP to be retrieved jointly with the T_{cir} measurements from adjacent scans.

3.16.9 Summary for IWP

IWP column bottom: 6 km (estimated from MLS radiative transfer model calculations).

The calculation of the bottom height of the IWP column depends on the tropospheric water vapor loading and on the IWP itself and is discussed in *Wu et al.* [2009].

Typical precision: 3 g/m^2 is the typical 1σ precision.

The precision for a particular measurement must be evaluated on a daily basis using the method described in the text.

Accuracy: 50% (estimated from comparisons with CloudSat)

Resolution: 60 km along track, 7 km across track (the volume of air sampled by MLS)

Valid IWP range: ≤200 g/m^2

This is the range where the stated precision, accuracy and resolution are applied. In this range MLS measurements can be quantitatively interpreted as the average IWP for the volume sampled. IWP values above this range, currently giving qualitative information on cloud ice, require further validation for quantitative interpretation.

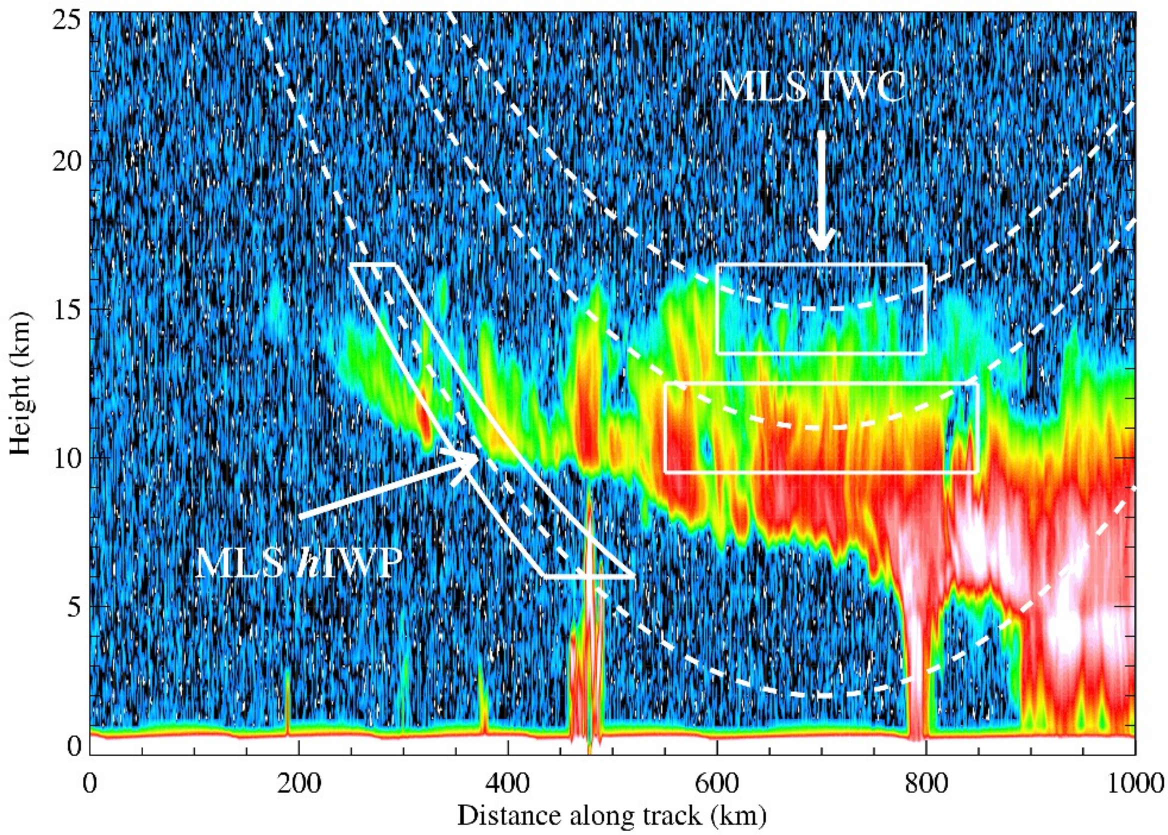

Figure 3.16.1: Diagram to illustrate the MLS IWC and IWP measurement. The dashed lines are the MLS tangential beams. At high tangent heights, the beams penetrate through the limb and become sensitive to a volume-averaged IWC, whereas at low tangent heights the MLS beams cannot penetrate through the limb due to strong gaseous absorption and become only sensitive to a partial slant column of IWP, with a shallow (~3°) angle, "hIWP". Note that the actual volume of the air represented by hIWP is centered ~300 km away from the tangent point, or ~2 profiles from the location of the nominal profile.

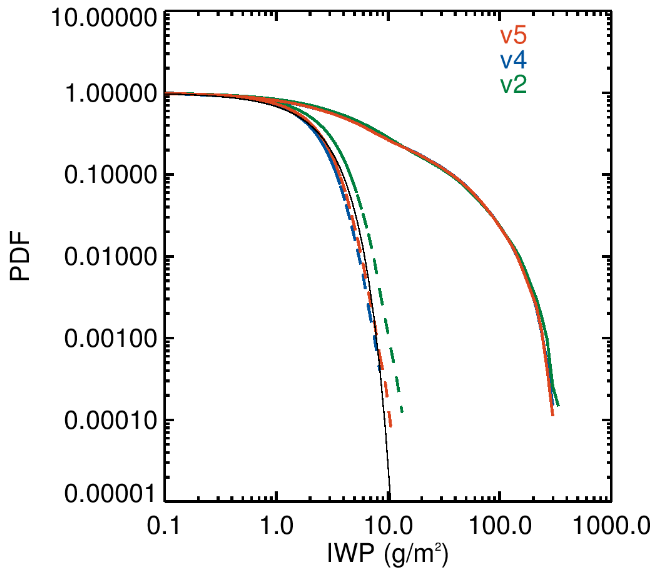

Figure 3.16.2: MLS v5, v4 and v2 IWP comparisons for July 2009. (a) Left: Probability density functions (PDF) (v5 (red), v4 (blue) and v2 (green)) with dashed lines showing the corresponding noise levels (obtained by folding the negative IWP values about the origin) and the thin black lines representing the gaussian error function. (b) Right: Scatter plot of IWP v5 vs v2 (black points) with a red line indicating the 1:1 line and a linear fit to the data shown as a blue line.

3.17 Nitrous Oxide (N_2O)

Swath name: N2O

Useful range: 100–0.46 hPa

Contact: Alyn Lambert, **Email:** <Alyn.Lambert@jpl.nasa.gov>

3.17.1 Introduction

N_2O standard product

The standard product for v5.0*x* N_2O is taken from the MLS "band 3" 190-GHz radiances (retrieved in the `NitrousOxide` phase) in order to provide a continuous data product (`N2O-NitrousOxide`) from launch. Previous versions (v3 and earlier) of the N_2O standard product relied on the "band 12" 640-GHz (`CorePlusR4B`) retrieval, however, as documented in the v4.2*x* data quality document, a noticeable reduction in quality of the band 12 radiance signals became evident during June-August 2013. Band 12 was finally turned off on August 6, 2013, and the data collected on and after 7 June 2013 for `N2O-640` are not recommended for scientific use.

During the MLS v5.0*x* development the opportunity was taken to address the problem of the high bias in the v4.2*x* 190-GHz N_2O product at 100 hPa, which has rendered this pressure level unsuitable for scientific use in all previous versions. For v5.0*x*, a separate retrieval phase for the N_2O product has been devised to improve the treatment of spectral "background" signals, in which the continuum absorption from O_2, N_2, and H_2O is modeled with an expected ν^2 dependence in frequency. The double sideband receiver folds together the upper frequency side band (containing the N_2O line) and lower frequency side band, thus making it impossible to disentangle the degree of interference between the continuum absorption and the N_2O line. The legacy 190 GHz N_2O data product (`N2O-190`), retrieved in the "CorePlusR2" phase (which retrieves water vapor and other 190-GHz products), is used by the MLS team purely for internal monitoring purposes and with v5.0*x* it is no longer intended for scientific use.

Unfortunately, including the sideband fraction offset developed for H_2O in the standalone N_2O retrieval phase did not alleviate the high bias in lower stratospheric N_2O. Accordingly, the decision was made to implement a sideband fraction correction that contains only the drift term, and not the offset term, for the N_2O-focused phase. The new N_2O retrieval phase ("N2O-NitrousOxide") uses the prelaunch sideband fraction values, but with the same drift correction derived from post-launch measurements of H_2O. The latter is necessary because without an imposed temporal sideband fraction drift, the UTLS N_2O does not display the expected trend upwards with time, resulting from the secular emissions increase seen in ground based observations. These changes are expected to affect the concentration bias but do not change the morphology of the MLS N_2O measurement. As reprocessing of the v5 dataset continues, planned comparisons with other N_2O observations (e.g., from ACE-FTS) will be used to re-validate the MLS N_2O product in the lower stratosphere

The 190-GHz N_2O data product in general shows slightly worse precision and resolution compared to the 640-GHz retrievals, although the 190-GHz precision is substantially better at 100–68 hPa. Data from `N2O-NitrousOxide` and `N2O-640` have been compared from launch until the end of band 12 operations. A persistent low bias over the pressure range 46 to 22 hPa peaking at −15% is seen in the `N2O-NitrousOxide` product compared to `N2O-640`. The biases are generally smaller than 5% from 100 to 68 hPa and 10% from 15 to 4.5 hPa (see Figure 3.17.1).

Other significant differences between the v5.0*x* `N2O-NitrousOxide` and `N2O-640` data such as the resolution, precision, recommended pressure levels, quality and convergence criteria are noted below.

The secondary v5.0*x* N_2O 640-GHz product is available for the period from launch until June 6, 2013 and stored in the `L2GP-DGG` files in the `N2O-640` swath. Details of the retrieval method and validation results are presented in [*Lambert et al.*, 2007].

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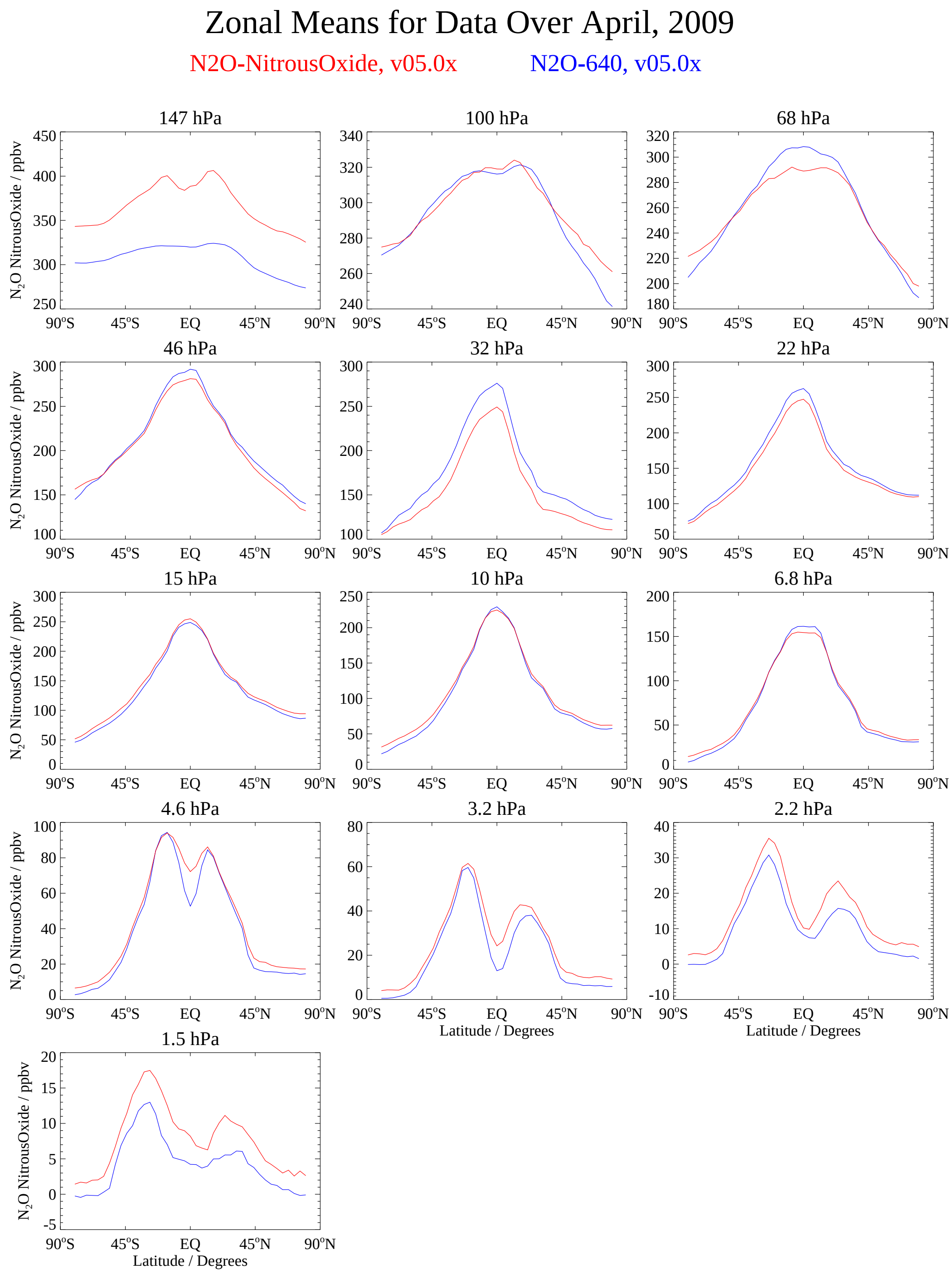

Figure 3.17.1: MLS v5.0x `N2O-NitrousOxide` and `N2O-640` comparison for April 2009

3.17.2 Resolution

The spatial resolution reported by the averaging kernel matrices is shown in Figures 3.17.2 for the 190 GHz measurements and 3.17.3 for the 640 GHz measurements (available in the `L2GP-DGG` files for data prior to June 6, 2013). For `N2O-NitrousOxide`, the vertical resolution is 5–8 km and the horizontal along-track resolution is 165–260 km. For `N2O-640`, the vertical resolution is 4–6 km and the horizontal along-track resolution is 330–600 km over most of the useful range of the retrievals.

The horizontal cross-track resolution is set by the 7 km width of the MLS 190-GHz field-of-view for all pressures. Note that the higher frequency MLS 640-GHz measurements have a narrower 3 km field-of-view. The longitudinal separation of the MLS measurements is 10°– 20° over middle and lower latitudes, with much finer sampling in polar regions.

3.17.3 Precision

Precision as defined here is the 1σ uncertainty in the retrieved value calculated by the Level 2 algorithms and has been validated against the scatter about the mean of coincident ascending/descending MLS profile differences. The estimated precision on a single retrieved profile given in Tables 3.17.1 and 3.17.2 varies with height from ~12–18 ppbv for `N2O-NitrousOxide` and ~12–25 ppbv for `N2O-640`.

3.17.4 Accuracy

The accuracy values given in Table 3.17.2 were obtained for both v4.2*x* N_2O products using the same detailed analyses presented for MLS `N2O-640` v2.2 data in *Lambert et al.* [2007] to quantify the systematic uncertainties associated with the MLS instrument calibration, spectroscopic uncertainty and approximations in the retrieval formulation and implementation. These systematics will be evaluated for v5.0*x* at a later date, but the estimates presented here for v4.2*x* are expected to be fairly representative.

3.17.5 Data screening

Pressure range (`N2O-NitrousOxide`): 100–0.46 hPa

Pressure range (`N2O-640`): 100–0.46 hPa

Values outside this range are not recommended for scientific use. In the upper stratosphere and lower mesosphere v5.0*x* N_2O requires significant averaging for useful signals, but see the note under "Artifacts" for issues at pressures below 0.1 hPa.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality (`N2O-NitrousOxide`): Only profiles whose `Quality` field is greater than 0.8 should be used.

A small fraction of `N2O-NitrousOxide` profiles (typically less than 1.5%) will be discarded via this screening.

Convergence (`N2O-NitrousOxide`): Only profiles whose `Convergence` field is less than 2.0 should be used.

A fraction of the `N2O-NitrousOxide` data (typically less than 0.5%) at this level will be discarded via this screening.

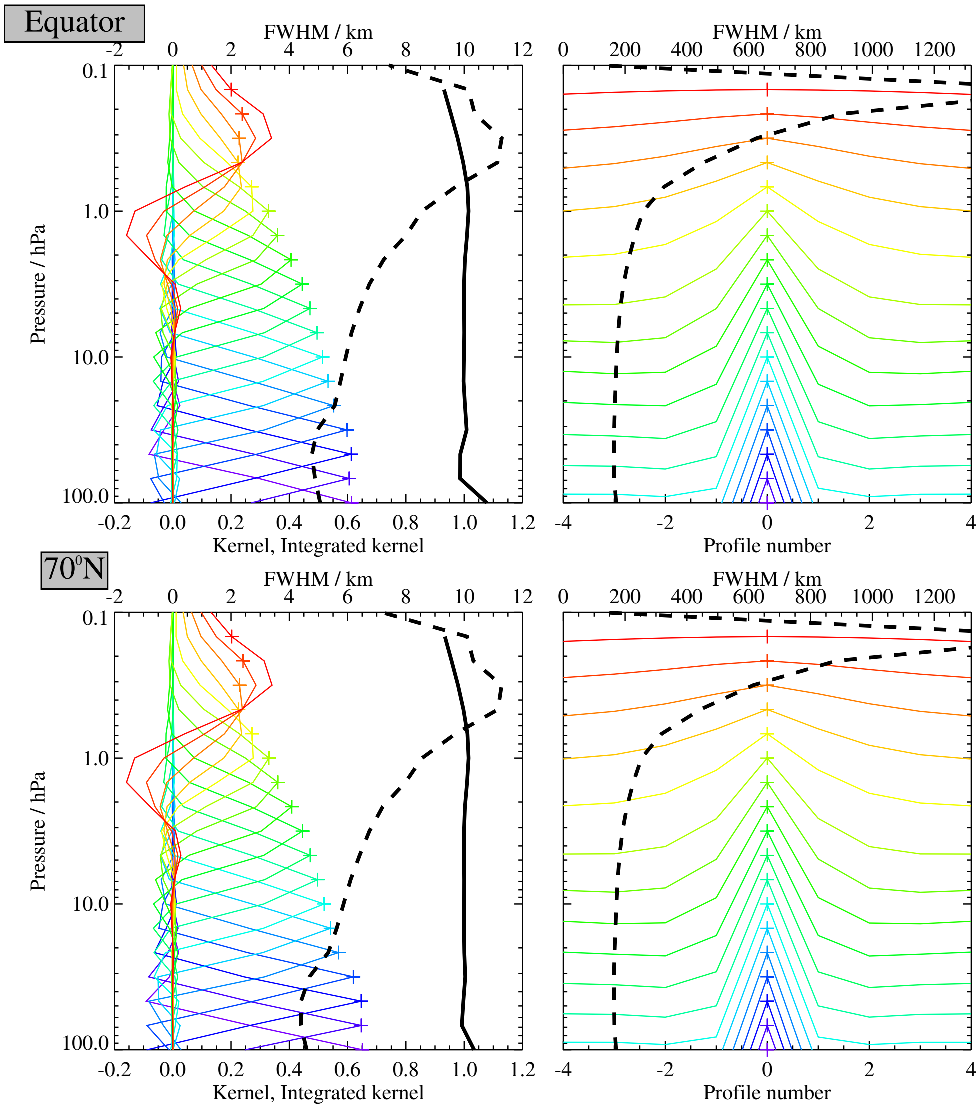

Figure 3.17.2: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x 190 GHz N_2O data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

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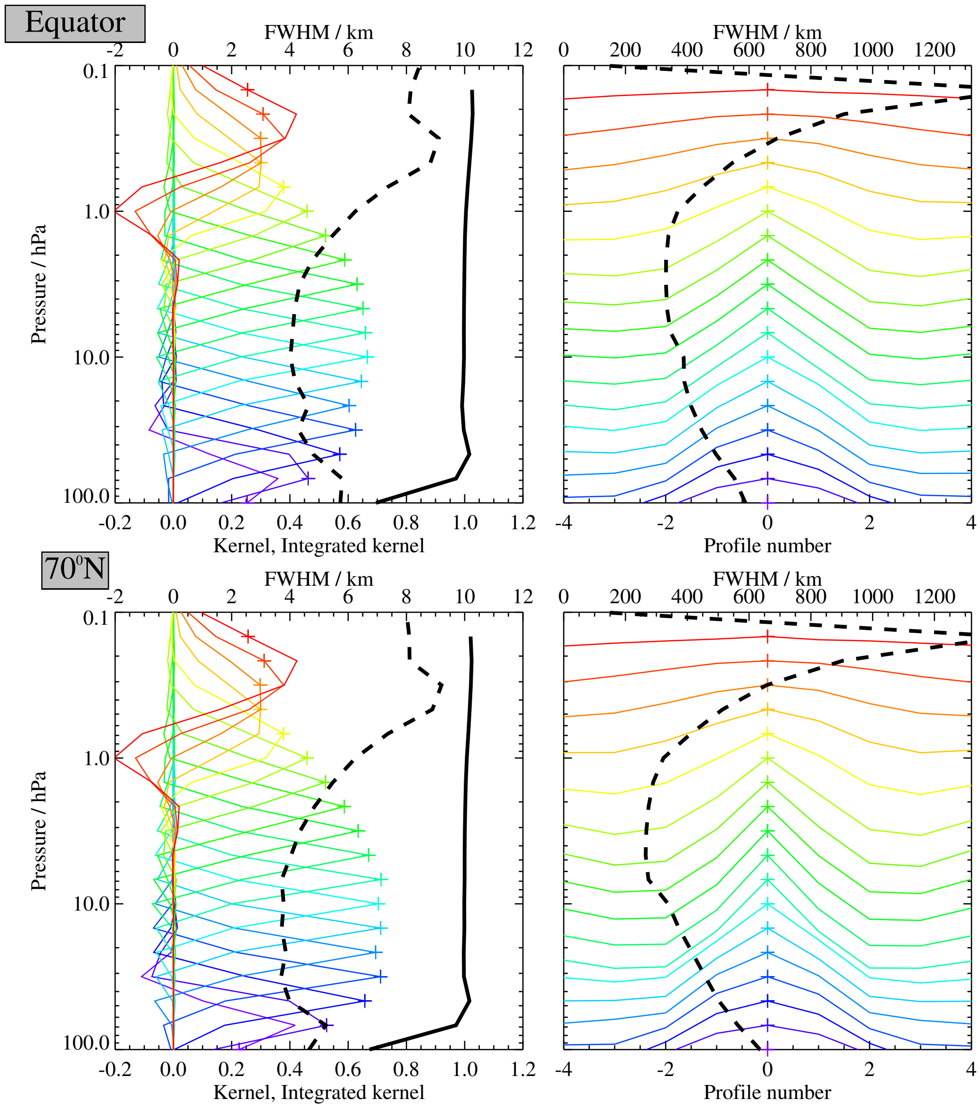

Figure 3.17.3: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x 640 GHz N_2O data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Quality (`N2O-640`): Only profiles whose `Quality` field is greater than 1.4 should be used.

A small fraction of `N2O-640` profiles (typically less than 1.5%) will be discarded via this screening.

Convergence (`N2O-640`): Only profiles whose `Convergence` field is less than 1.01 should be used.

A fraction of the `N2O-640` data (typically less than 0.5%) at this level will be discarded via this screening.

Clouds: Clouds have little impact on the N_2O products at the recommended pressure levels. Ignore status bit 16 (high cloud) or bit 32 (low cloud) indicating the presence of clouds. See artifacts for more details.

3.17.6 Artifacts

There are occasional outliers at the highest presure levels in `N2O-NitrousOxide` and `N2O-640` products. As with v4.2*x*, very thick clouds in the tropics produce a low rate of artifacts in the v5.0*x* N_2O products since improvements in the handling of radiances affected by clouds have reduced the frequency of outliers compared to older versions. The cloud bits of the `Status` field are too blunt a tool to identify these rare cases, needlessly discarding reasonable data. Screening using the convergence and quality fields (see above) is recommended to remove the majority of these data points.

The retrieval restricts N_2O values to be greater than −40 ppbv (approximately three times the retrieval noise level in the recommended pressure range) in order to prevent problems in the minimization search process. The low bound is applied at all levels, but it is only evident in the data for pressures less than 0.1 hPa, where the vertical smoothing is relaxed and the retrieval noise becomes comparable to the magnitude of the low bound value. Accordingly, statistical averaging of the data (zonal means or longer time periods) cannot be applied successfully for pressures at and less than 0.1 hPa as the −40 ppbv hard limit introduces a positive bias in any average.

3.17.7 Review of comparisons between MLS N_2O versions and other datasets

Average values for v5.0*x* 190-GHz N_2O are substantially smaller and more realistic than in previous versions for the 100 and 68 hPa pressure levels. For pressures smaller than 68 hPa (i.e., at altitudes higher than this pressure surface) differences are within a few percent (see Figure 3.17.4).

Average values for v5.0*x* 640-GHz N_2O are 20% larger than in v2.2 for the 100 hPa pressure level, up to 10% smaller at the 46–32 hPa levels, and within 5% for pressures greater than 22 hPa (see Figure 3.17.5). Differences between v5.0*x* 640-GHz N_2O and v4.2*x* are less than 10% at all levels.

Apart from the differences noted above, the MLS v5.0*x* 640 GHz N_2O is similar to the MLS v2.2 product described and validated in *Lambert et al.* [2007]. Comparisons of v2.2 640 GHz N_2O with coincident measuremements by ACE-FTS, Odin/SMR, and Envisat/MIPAS and balloon borne observations are shown in *Lambert et al.* [2007]. A revised validation paper for N_2O is not planned and users are encouraged to read *Lambert et al.* [2007] for more information.

3.17.8 Desired improvements for future data version(s)

Retrievals of N_2O to pressures greater than 100 hPa *may* be possible in later versions from the 190-GHz observations.

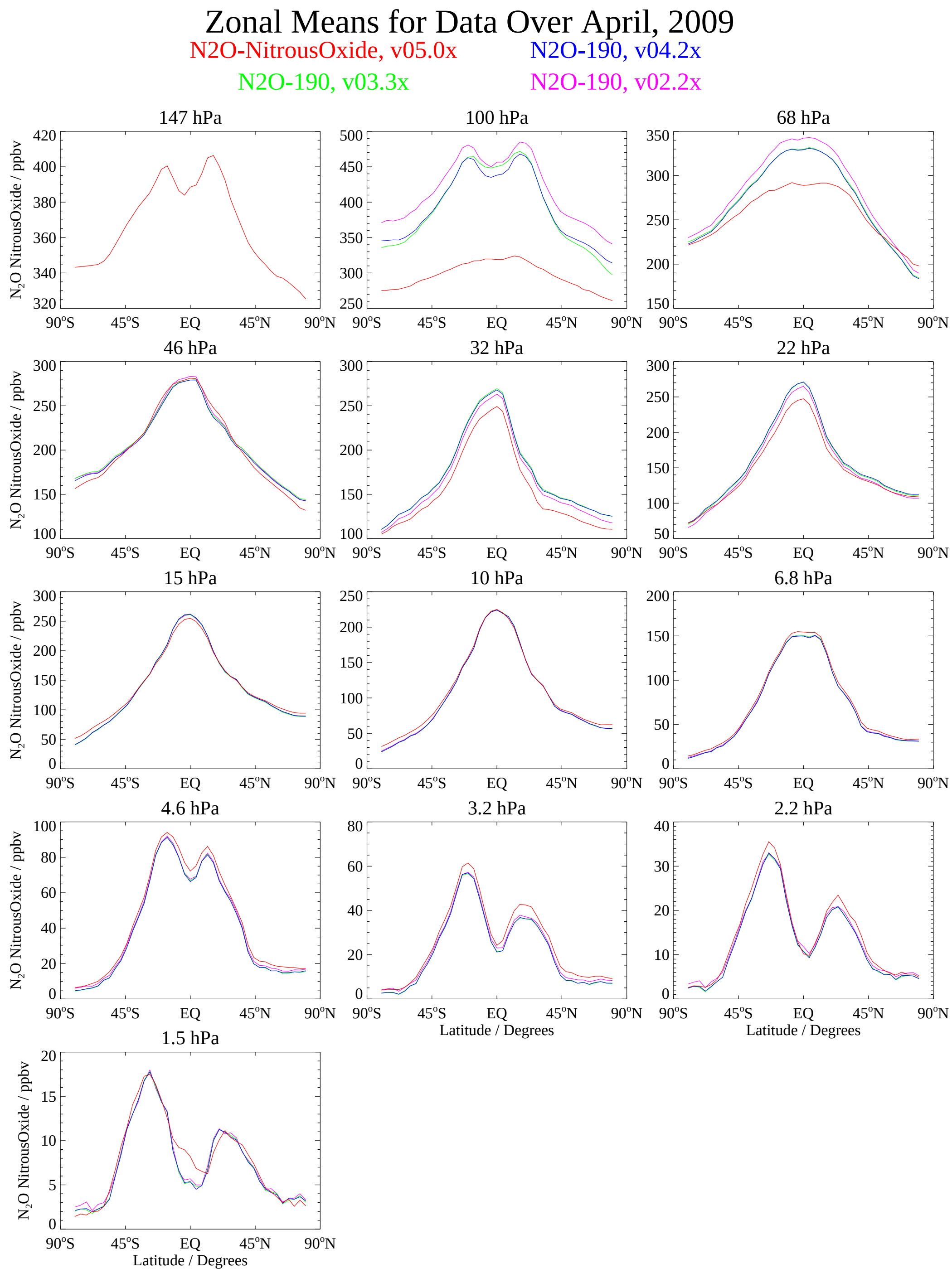

Figure 3.17.4: MLS v5.0 190-GHz N_2O compared to v2.2, v3.3 and v4.2 for April 2009

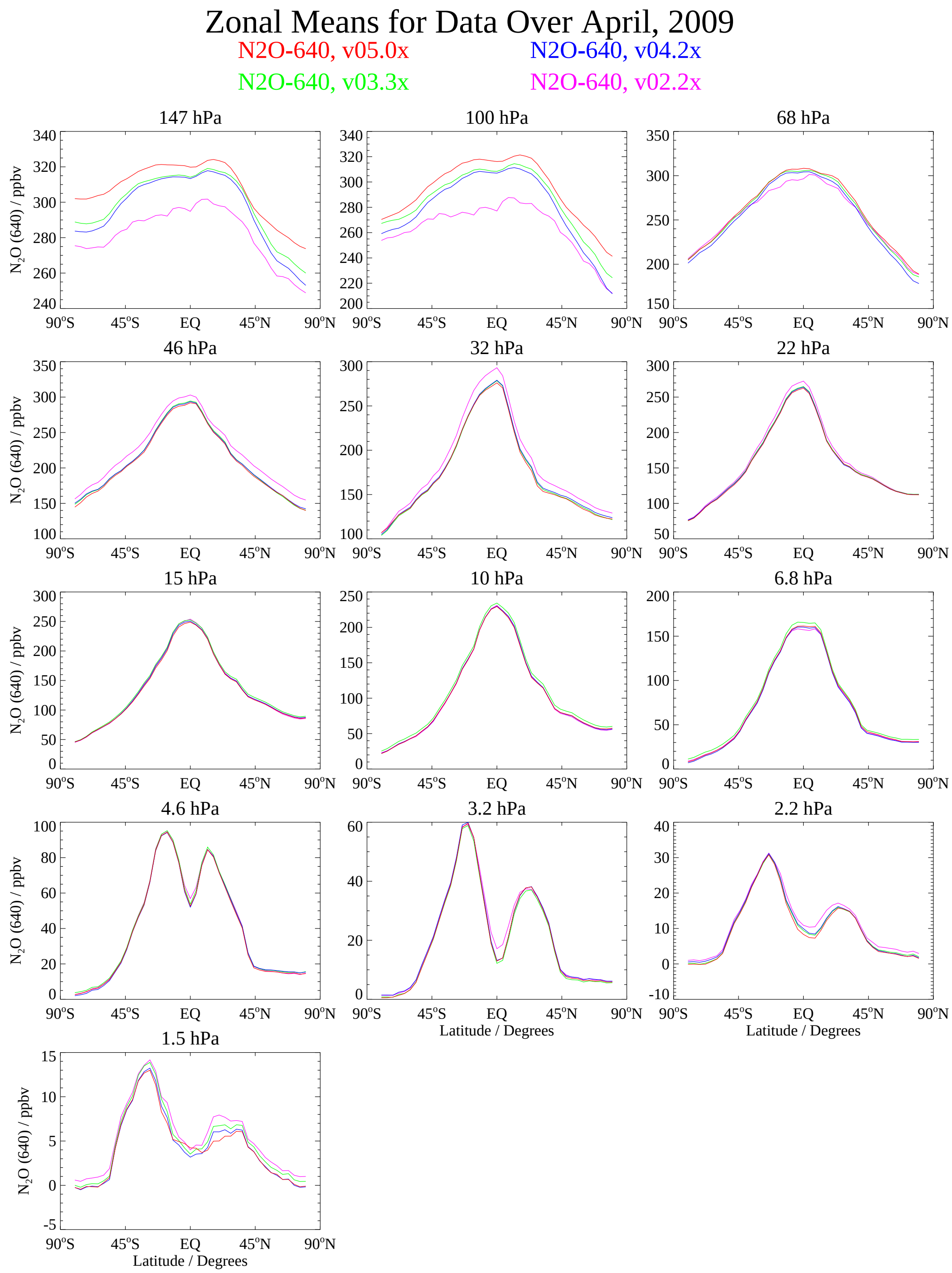

Figure 3.17.5: MLS v5.0 640 GHz N_2O compared to v2.2, v3.3 and v4.2 for April 2009

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

Table 3.17.1: Summary of MLS v5.0x N_2O (`N2O-NitrousOxide`) product.

Region	Resolution Vert. × Horiz.	Precision[a]		Accuracy		Comments
hPa	km	ppbv	%	ppbv	%	
≤0.33	—	—	—	—	—	Unsuitable for scientific use
0.46	11.0 × 450	14	>100	2	17	
0.68	9.7 × 325	16	>100	2	11	
1.0	8.6 × 260	17	>100	2	10	
2.2	7.2 × 210	18	61	4	9	
4.6	6.4 × 185	16	22	5	7	
10	6.0 × 175	15	11	6	5	
22	5.6 × 165	14	8	13	7	
46	4.8 × 165	12	6	24	10	
68	4.9 × 165	12	5	30	11	
100	5.1 × 170	12	4	55	19	
147	—	—	—	—	—	Unsuitable for scientific use
≥215	—	—	—	—	—	Unsuitable for scientific use

[a]Precision on individual profiles

Table 3.17.2: Summary of MLS v5.0x N_2O (`N2O-640`) product.

Region	Resolution Vert. × Horiz.	Precision[a]		Accuracy		Comments
hPa	km	ppbv	%	ppbv	%	
≤0.33	—	—	—	—	—	Unsuitable for scientific use
0.46	8.8 × 550	12	>100	1	16	
0.68	7.4 × 450	13	>100	2	12	
1.0	6.3 × 370	14	>100	2	10	
2.2	4.8 × 330	15	49	3	7	
4.6	4.2 × 335	14	18	5	7	
10	4.0 × 390	14	11	12	9	
22	4.6 × 410	15	9	21	11	
46	4.8 × 495	17	8	36	15	
68	5.8 × 555	21	8	32	12	
100	5.7 × 590	25	9	47	16	
147	—	—	—	—	—	Unsuitable for scientific use
≥215	—	—	—	—	—	Not retrieved

[a]Precision on individual profiles

3.18 Ozone (O_3)

Swath name: O3

Useful range: 261–0.001 hPa

Contact: Lucien Froidevaux (stratosphere/mesosphere),
Email: <Lucien.Froidevaux@jpl.nasa.gov>
Michael Schwartz (upper troposphere), **Email:** <Michael.J.Schwartz@jpl.nasa.gov>

3.18.1 Introduction

The most significant difference for the MLS ozone retrievals is that v5.0*x* uses a more accurate non-linear radiative transfer model (in place of an approximate linear model) for the digital autocorrelator (DAC) channels covering the center of the 236-GHz ozone line. This changes (and should improve) the ozone retrieval results for pressures less than about 0.02 hPa. The changes are illustrated in Figure 3.18.1 for April, 2019, for the 30° N to 60° N latitude range. While there is currently no proper validation of MLS ozone at this higher altitude range, there is clearly sensitivity to the nighttime ozone maximum mixing ratio near 0.001 hPa. The ozone retrieval now uses a larger value for the *a priori* errors in this topmost height range, so as to provide less dependence on the *a priori* values, also shown in the Figure (at much reduced abundances compared to retrieved values near 0.002 to 0.001 hPa). Thus, further analyses of v5.0*x* MLS ozone in this extended range are now enabled. In fact, a recent analysis [*Lee and Wu*, 2020] has shown that the v4.2*x* ozone retrieval already had enough radiance sensitivity in this altitude range to show strong dependence on the 11-year solar cycle variations (as for carbon monoxide).

As is the case with previous data versions, the v5.0*x* standard O_3 product is taken from a retrieval using 240-GHz radiances, providing sensitivity from the upper troposphere to high altitudes (into the thermosphere, with v5.0*x* retrievals). In v5.0*x*, as in v4, there is an optimized retrieval phase for the production of the O_3 standard product prior to the phase that uses 240-GHz radiances to produce the standard carbon monoxide and nitric acid products. Table 3.18.1 summarizes typical O_3 resolution, precision (random uncertainty), and accuracy (systematic uncertainty) estimates versus pressure. Papers describing detailed validation of the MLS v2.2 product and comparisons with other data sets were published in a special Aura validation issue of the *Journal of Geophysical Research*, see [*Froidevaux et al.*, 2008b; *Jiang et al.*, 2007; *Livesey et al.*, 2008]. In the stratosphere, v5.0*x* ozone profiles are very similar to those of previous data versions including v4.2*x*. While stratospheric ozone results from the above references will generally hold, we plan to provide validation updates in the future regarding v5.0*x* ozone for different height regions and specific parts of the globe. Initial documentation of changes, improvements, and issues with v5.0*x* data are discussed here, including data screening criteria. Recommended v5.0*x* data screening is again based on thresholds for `Status`, `Quality`, and `Convergence`.

Vertical oscillations in the UTLS and sensitivity to thick clouds were reduced in v4.2*x* ozone through changes in the spectral form used to model cloud impacts on MLS radiances, through tightening of vertical smoothing at pressures greater than 67 hPa, and by retrieving a spectrally-flat baseline over the ozone band for each limb view to better account for cloud inhomogeneity. Further changes in stratospheric ozone between v4.2*x* and v5.0*x* are generally quite small, as little was changed in the retrieval system.

Some higher accuracy forward model calculations were carried out for v5.0*x*, and this had a small impact in the UTLS, with some results slightly better, and some slightly worse than before (see further below), depending on the time period and latitude region. These changes are within the accuracy estimates.

In addition to the swath `O3`, which gives the O_3 profile on 55 pressure surfaces, the `L2GP-O3` files con-

Help Overview Table BrO S T CH_3Cl S T CH_3CN S T CH_3OH S T ClO S T CO S T GPH S T H_2O S T HCl S T HCN S T HNO_3 S T HO_2 S T HOCl S T IWC S T IWP S T N_2O S T O_3 S T OH S T RHI S T SO_2 S T T S T Lvl 3

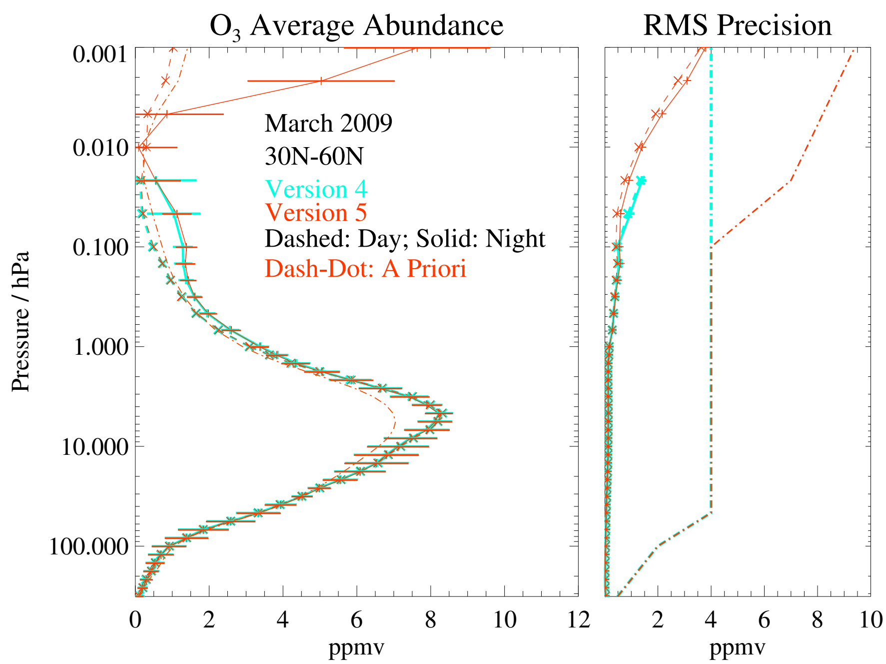

Figure 3.18.1: Left panel: Zonal mean ozone abundances from v5.0x (red) and v4 (cyan) for April, 2019, and 30°N to 60°N, for both daytime (dashed) and nighttime (solid) cases, corresponding to solar zenith angles below 90° or above 100°, respectively. The average (v5.0x) a priori values for this case are also shown (as a dash-dot curve), and day and night values here are essentially identical. The v5.0x a priori values differ somewhat from the a priori values used in previous versions, as a result of changes in the climatological model currently used for this purpose, but this is not the point we wish to illustrate here. We also show the standard deviations associated with the monthly means as error bars, to illustrate that there is a significant amount of noise at high altitude (see also the single-profile precisions in the right panel). Right panel: The RMS precisions (random uncertainty estimates from Level 2) are displayed as a function of pressure for the same region and month as the left panel. The a priori errors are illustrated by the dash-dot curves, with changes between the two versions only showing at the highest altitudes. There is now slightly better sensitivity (smaller values of the random uncertainties) in the upper mesosphere (and above the topmost v4.2x recommended pressure level of 0.02 hPa).

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

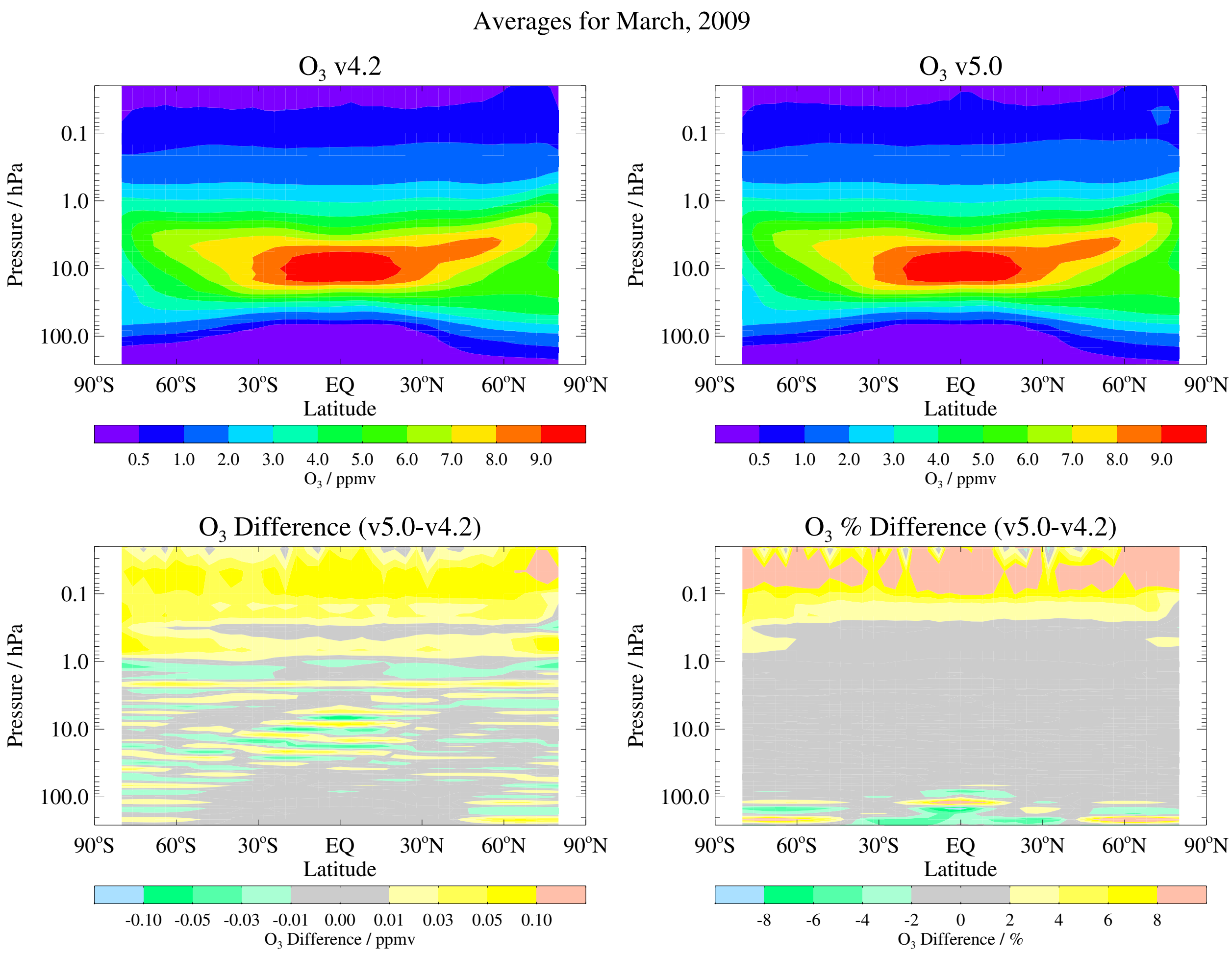

Figure 3.18.2: Zonal averages for stratospheric and mesospheric MLS ozone profiles during March, 2009, showing the MLS v4 ozone mixing ratio contours versus latitude (top left panel), the v5.0x contours (top right panel), and their differences in ppmv (v5.0x minus v4, bottom left panel) and percent (v5.0x minus v4 versus v4, bottom right panel).

tain a swath, `O3 column`, which is the integrated stratospheric column down to the thermal tropopause (WMO definition) calculated from MLS temperatures. The MLS temperature profiles from which the WMO tropopause is determined are not screened per the instructions of section 3.22; users may wish to reject ozone columns for which standard screening rejects (a small fraction of) the corresponding temperature profiles.

3.18.2 Comparison of v5.0*x* with past data versions

The vertical retrieval grid has not changed from v4.2*x*; between 316 hPa and 1 hPa, v5.0*x* ozone profiles are retrieved on 12 surfaces per decade, with a coarser retrieval grid at higher altitudes.

Table 3.18.1 summarizes resolution, precision, and accuracy estimates.

Figure 3.18.2 shows zonally-averaged stratospheric and mesospheric ozone field comparisons between v4.2*x* and v5.0*x* for the (full) month of March, 2009, for properly screened profiles only; mean differences (ppmv and percent) are also shown. Similar plots focusing on the UTLS are provided in Figure 3.18.3. Average stratospheric ozone abundances (monthly zonal means) have typically not changed by more than 1 to 2% for pressures less than 100 hPa, and have changed by only slightly more (in %)

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

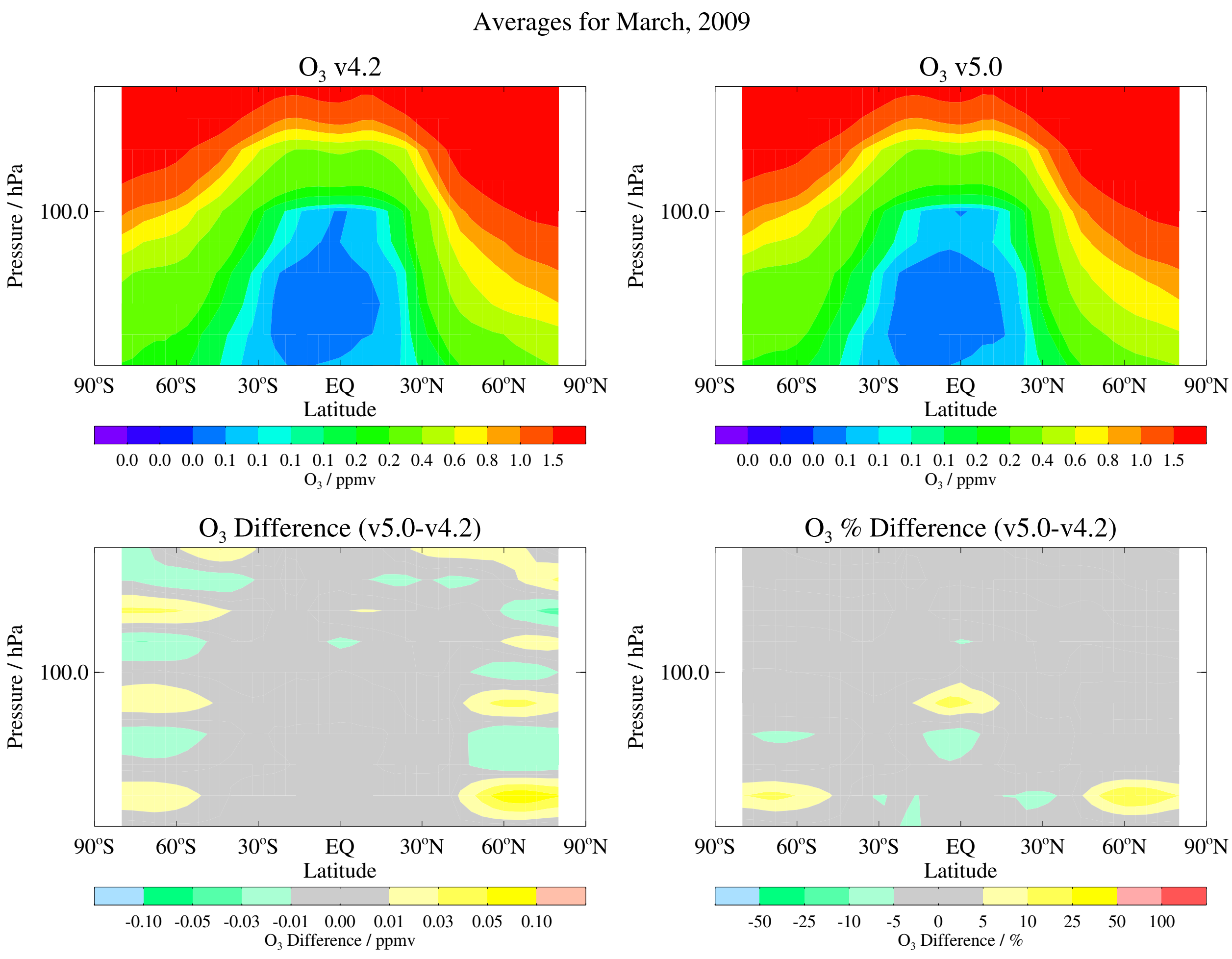

Figure 3.18.3: As Figure 3.18.2, but for the UTLS region, plotted here from 261 to 46 hPa. For other months or years, we have generally found similar or slightly smaller differences.

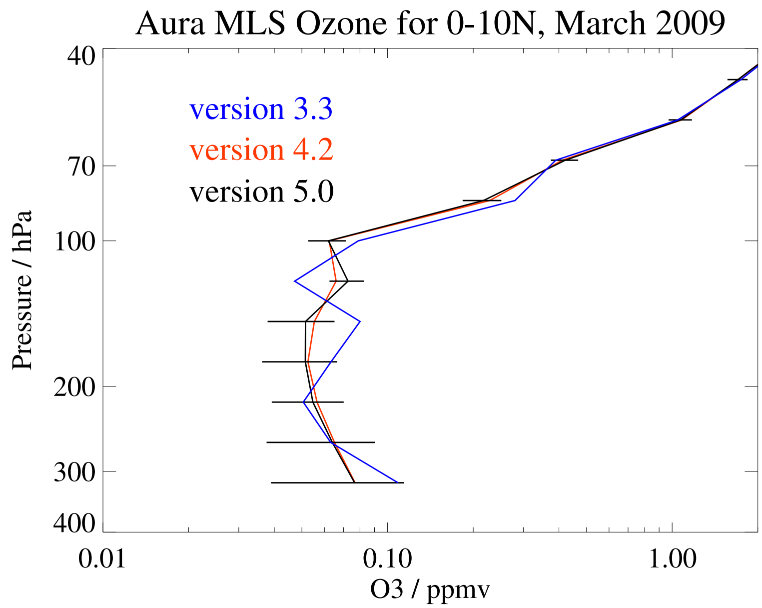

Figure 3.18.4: Zonal means from equator to 10°N during March, 2009, showing the average behavior of ozone profiles for MLS v3, v4, and v5.0x, as indicated by the color-coded legend.

at pressures larger than 100 hPa. Average v5.0*x* values from 0.1 to 0.02 hPa are larger than v4.2*x* data by 5 to 10%. We show average UTLS profiles during March, 2009 from three data versions for 0°– 10°N in Figure 3.18.4. Version 5 is very close to version 4 in terms of the vertical oscillations in these tropical profiles. For certain months, there is a slightly larger oscillation in v5 ozone, but there is also a slight decrease (typically only by a few percent) in the tropical v5 data from about 215 to 261 hPa, in comparison to v4. This latter change goes in the right direction, as we know that average MLS ozone is biased high in this region versus ozonesonde profiles. This slight improvement is mainly the result of a more accurately calculated forward model (in the ray tracing calculations) in MLS version 5. None of these changes are outside the accuracy (systematic error) estimates for the MLS profiles. These estimates are provided in Table 3.18.1, but based on v4 sensitivity tests. Updated (v5) accuracy estimates will be provided at a later date, but changes relative to v4.2*x* are expected to be small except at the top of the retrieval, where better use of line-center radiances has allowed the retrieval to be extended to lower pressures.

Ozone Columns

A stratospheric column swath, using a tropopause derived from MLS temperatures, is calculated by the v5.0*x* O_3 retrieval. Changes in the MLS stratospheric ozone columns between v4.2*x* and v5.0*x* are quite small; daily zonal averages are typically within one percent.

3.18.3 Resolution

Typical resolution values are provided in the summary Table 3.18.1, as derived from the full width at half-maximum of typical averaging kernels in the vertical and horizontal (along-track) coordinates, shown in Figures 3.18.5 and 3.18.6, for the whole vertical range, and the UTLS, respectively. The cross-track resolution is set by the 6 km width of the MLS 240 GHz field of view. Daily longitudinal separation of MLS measurements, set by the Aura orbit, is 10°– 20° over middle and lower latitudes, with much finer sampling at the highest latitudes sampled in each hemisphere.

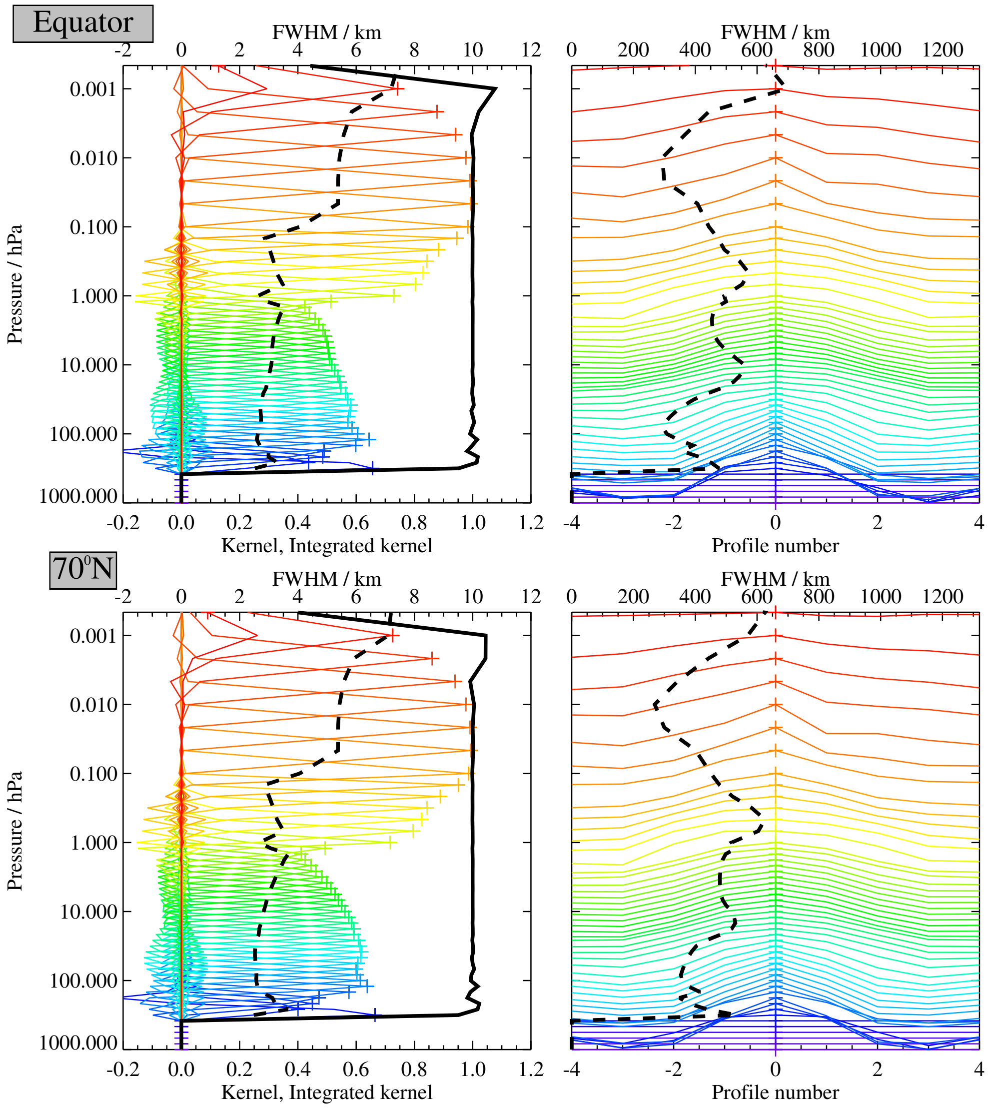

Figure 3.18.5: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x O_3 data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO CH3Cl CH3CN CH3OH ClO CO GPH H2O HCl HCN HNO3 HO2 HOCl IWC IWP N2O O3 OH RHI SO2 T Lvl 3

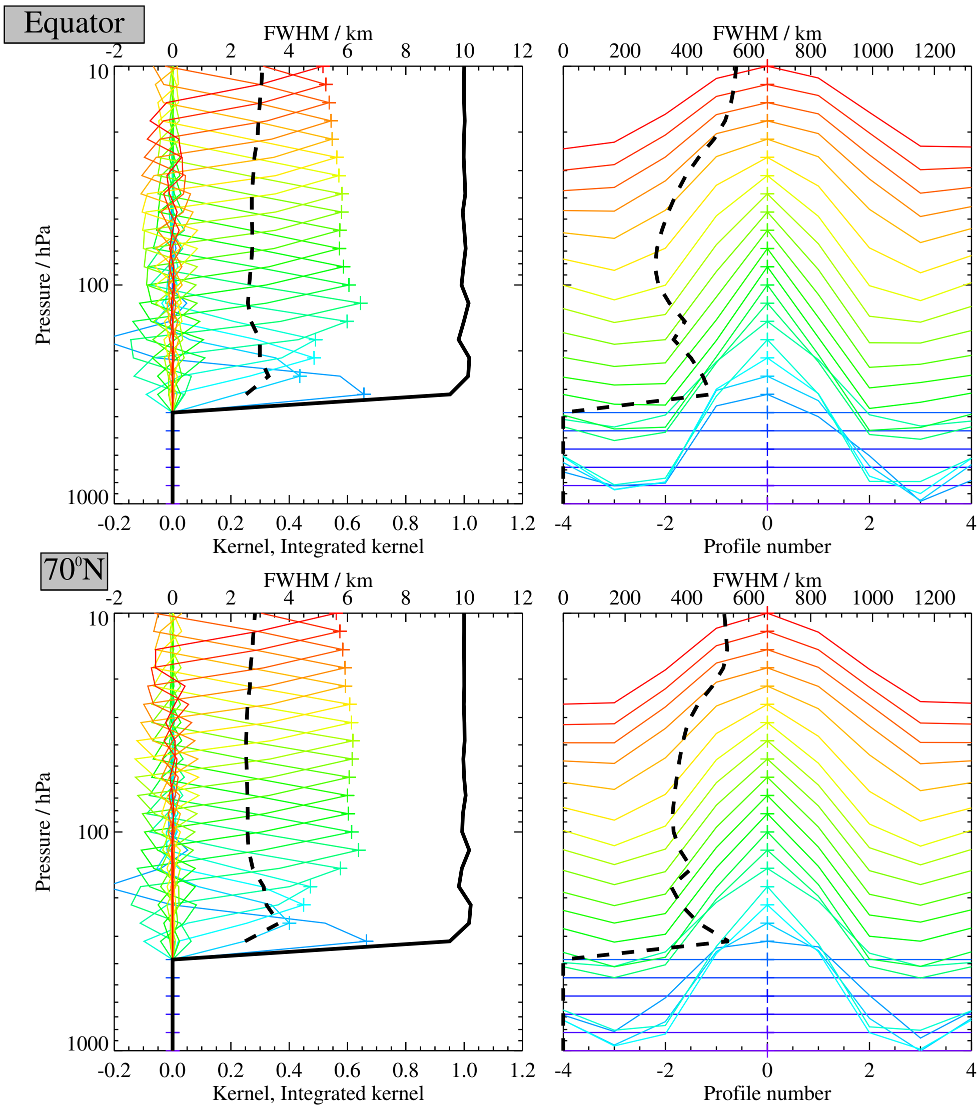

Figure 3.18.6: As for Figure 3.18.5 but zooming in on the upper troposphere and lower stratosphere region.

3.18.4 Precision

As found previously, the Level 2 precision values are often slightly lower than the scatter observed in a narrow latitude band centered around the equator (where atmospheric variability is expected to be small) or obtained from a comparison between ascending and descending coincident MLS profiles.

Negative precision values for ozone sometimes occur at the largest and smallest pressure values within the recommended range, which has been extended to upper mesospheric and thermospheric pressures in v5.0*x*, as mentioned earlier. Such flags on the precision values indicate that there is quite a significant influence from the *a priori*, although some MLS information can exist in these cases also. Caution is required if one wants to include such profile portions in scientific analyses, and our default recommendation is to ignore these values.

Column values

As for v4 data, the estimated precisions for the v5.0*x* MLS column ozone abundances down to pressures of 100 to 215 hPa are 2% or less. The typical empirical precision in the columns based on (1σ) variability in the tropics is 2 to 3%.

3.18.5 Accuracy

The accuracy estimates shown in Table 3.18.1 are from a v5 analysis which propagated estimated systematic errors in MLS calibration, spectroscopy, etc., through the (v5.0*x*) measurement system. The values shown here are intended to represent 2σ estimates of accuracy. Comparison of MLS O_3 with well-established data sets shows no evidence of significant biases overall, although the oscillations in the UTLS at low latitudes lead to some systematic effects which can reach 20–40%, depending on the pressure level. For more details, see the MLS validation papers by *Froidevaux et al.* [2008b], *Jiang et al.* [2007], and *Livesey et al.* [2008], as well as references therein. More recent references relevant to MLS ozone are available on the MLS website under "Publications". For validation purposes, see, in particular, the comprehensive work by *Hubert et al.* [2016] (more related information further below). In recent years, validation studies have focused more on longer-term changes or drifts (with good stability being observed versus other reliable measurements) and on the UTLS region. Validation updates are to be expected for v5.0*x*, after the multi-year dataset has been reprocessed.

Column values

Sensitivity tests using systematic changes in various parameters that could affect the accuracy of the MLS retrievals lead to possible biases (2σ estimates) of about 4%, as an estimated accuracy for the MLS column values (from integrated MLS ozone profiles down to 100, 147, and 215 hPa). This estimate is still expected to hold for v5 data. See the validation papers (and subsequent ozone-related publications, e.g., available from the MLS website) for results on column ozone comparisons versus satellite, sonde, and lidar data.

3.18.6 Data screening

Pressure range: 261–0.001 hPa.

Values outside this range are not recommended for scientific use. Data at 0.00046 hPa represents a total column at and above that pressure level. Scientific use of these 0.00046 hPa data may be possible, but requires consultation with the MLS team.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality: Only profiles whose `Quality` field is greater than 1.0 should be used.

Convergence: Only profiles whose `Convergence` field is less than 1.03 should be used.

Clouds: Scattering from thick clouds can lead to more systematic effects in the UTLS.

Most of the affected profiles are removed by the `Quality` and `Convergence` screening recommendations (although `Convergence` issues occur only rarely).

One should *reject* profiles with odd `Status` *or* even `Status` profiles with `Convergence` above the convergence threshold *or* `Quality` below the quality threshold. Conversely, one should *keep* profile values with even status *and* good `Convergence` *and* good `Quality`. These criteria typically remove 1 to 2 % of global daily data, with tropical latitudes showing somewhat larger data removal fractions of about 5%. This screening generally maintains sufficient coverage for a near-complete daily map (for any given day), even in the UTLS.

Compared to data screening recommendations for v4.2*x*, the screening of v5.0*x* data typically removes slightly fewer ozone profiles on a typical day, but this difference is only a fraction of a percent.

3.18.7 Review of comparisons with other datasets

Comparisons of MLS ozone with other ozone observations have indicated general agreement at the 5–10 % level with stratospheric profiles from a number of comparisons using satellite, balloon, aircraft, and ground-based data. A high MLS v2.2 bias at 215 hPa had been observed in some comparisons versus certain ozonesonde and satellite datasets. Such high biases were reduced in version v4.2*x*, with additional smaller reductions in the v5.0*x* ozone values. We have found that latitudinal and temporal changes observed in various correlative datasets are well reproduced by the MLS ozone product. Intercomparisons of a large variety of ozone measurements by satellite instruments were provided by *Tegtmeier et al.* [2013], as part of the analyses produced by the SPARC Data Initiative; the Aura MLS ozone values compare quite favorably to the multi-instrument mean values as well as to SAGE II ozone. The temporal stability of the Aura MLS ozone dataset has been shown to be very good, in comparison to lidar datasets (*Nair et al.* [2012]). The work by *Hubert et al.* [2016] includes both the lidar network and the ozonesonde network as references for a comprehensive satellite data intercomparison study. The latter authors show that average biases between MLS and latitudinally-binned data from lidar and ozonesonde sites across the globe is typically within 5% or better, with poorer behavior (known vertical oscillations) at low latitudes in the UTLS. In terms of drifts, the Aura MLS ozone dataset is shown (in the above work) to be “very stable”, with SAGE-II being the only other dataset to gain that characterization. MLS exhibits drifts with respect to the ground-based networks that fall within 1.5 to 2% per decade, with zero drift encompassed by the error bars (i.e. non-significant drifts), at least in the middle stratosphere. The Aura MLS data, in combination with older datasets, provides a critical tool for the study of global O_3 in a changing climate and into the O_3 recovery period, as the total abundance of anthropogenic ozone depleting substances continues to decline.

3.18.8 Artifacts

Oscillations in UTLS ozone: While significant reduction in vertical oscillations in the UT ozone retrieval was accomplished in v4.2*x*, oscillations are still evident in v4.2*x* and v5.0*x*, particularly at low latitudes. We have performed studies with different *a priori* values, and have not found a satisfactory resolution of this issue for now. It is possible that the retrieval grid is slightly too fine,

Table 3.18.1: Summary for MLS ozone

Pressure / hPa	Resolution Vert. × Horiz.	Precision[a] ppmv	%	Accuracy[b]	%	Comments
≤ 0.0005	—	—	—	—	—	Unsuitable for scientific use
0.001	7 × 650	3.4	> 40	0.9	30	Requires averaging
0.002	6 × 450	2.5	> 40	0.4	20	Requires averaging
0.005	5.5 × 350	1.7	> 200	0.3	25	Requires averaging
0.01	5.5 × 300	1.1	> 500	0.1	100	Requires averaging
0.02	5.5 × 300	0.7	> 100	0.15	40	Requires averaging
0.05	5.5 × 400	0.4	50	0.1	15	
0.10	4 × 450	0.4	40	0.1	10	
0.21	3 × 500	0.4	30	0.1	8	
0.46	3.5 × 600	0.3	20	0.2	10	
1	3× 500	0.2	7	0.3	10	
2	3.5 × 500	0.15	3	0.3	7	
4.6	3 × 500	0.15	2	0.4	7	
10	3 × 500	0.1	2	0.4	6	
21	2.5 × 400	0.1	2	0.25	5	
46	2.5 × 350	0.06	3	0.2	8	
68	2.5 × 350	0.04	4	0.1	7	
100	2.5 × 300	0.04	20–30	[+0.005 + 7%]		
150	2.5 × 400	0.03	5–100	[+0.005 + 7%]		
215	3 × 400	0.02	5–100	[+0.01 + 10%]		
261	3.5 × 450	0.03	5–100	[+0.02 + 10%]		See note [c]
316	2.5 × 500	0.04	—	—	—	Not recommended
1000–464	—	—	—	—	—	Not retrieved

[a]Precision on individual profiles

[b]Primarily as estimated from systematic uncertainty characterization tests (based on a full day of retrieval perturbations). Stratospheric values are expressed in ppmv with a typical *equivalent* percentage value quoted. 261–100 hPa accuracies are the sum of the ppmv *and percentage* uncertainties; the ppmv terms arise from observed average positive biases in the MLS values relative to climatological tropical sonde data.

[c]Positive bias in the UT, but the mean annual variation is nevertheless well behaved versus tropical sonde data.

which is something for future investigations; we are also reaching the limit of possible retrieval remedies to the net impact of (known and unknown) systematic uncertainties on the MLS ozone retrievals. Further characterization of MLS UTLS data is warranted in order to more fully understand these data limitations; however, these oscillations are not expected to significantly impede studies of long-term trends.

3.19 Hydroxyl Radical (OH)

Swath name: `OH`

Useful range: 32–0.0032 hPa

Contact: Luis Millán, **Email:** `<Luis.F.Millan@jpl.nasa.gov>`

3.19.1 Introduction

The MLS THz radiometer is dedicated to measuring OH in the 2.5 THz spectral region. A description of OH data quality, precision and systematic errors for an earlier version, v2.2, is given in *Pickett et al.* [2006b]. The validation studies are described in *Pickett et al.* [2008] and *Wang et al.* [2008]. While the OH data quality is generally similar between v2.2 and v3.x, there were significant improvements in v4.x inherited to v5.0*x*. Previous to v3.x, OH data near the mesospheric density peak, ∼0.032 hPa, often show considerable amount of data flagged with negative precision, indicating strong influence of *a priori* information, particularly in the summer hemisphere (or tropics when near the equinox) and sometimes causes gaps in zonal mean time series. Starting with v4.x, the software resolves this issue by fixing the overly tight `a priori` constraints. The resulting mesospheric OH data are less noisy and generally have somewhat larger values than previous versions for the problematic seasons/latitudes. Another improvement is the smaller bias at 10–15 hPa. Therefore, the day-night correction for bias is only required for pressure levels at 21 and 32 hPa. Note that users may notice more zig-zags in nighttime mesospheric OH vertical profiles. This is a side effect of fixing the possible positive bias introduced by tight lower limits set in previous version retrievals.

The estimated uncertainties, precisions, and resolution for v5.0*x* OH are summarized in Table 3.19.1.

3.19.2 Resolution

Figure 3.19.1 shows the OH averaging kernel for daytime and nighttime at 35°N. The reason to separate daytime and nighttime is that the largest natural variability in OH is diurnal. The vertical resolution is slightly different between day and night. The nighttime resolution is sufficient to allow the study of (for example) the "nighttime OH layer" around 82 km. The vertical width of the averaging kernel for pressures greater than 0.01 hPa is 2.5 km. The horizontal width of the averaging kernel is equivalent to a width of 1.5°(165 km distance) along the orbit. The changes in vertical resolution above 0.01 hPa are due mainly to use of a faster instrument vertical scan rate for tangent heights above 70 km. The horizontal resolution across track is 2.5 km. The averaging kernel and resolution for high and low latitudes are very similar to Figure 3.19.1 for most pressure levels. At the topmost two pressure levels, 0.0046 hPa and 0.0032 hPa, the vertical resolution is slightly better at the equator than at 70°N.

3.19.3 Precision

A typical OH profile and the associated precisions (for both v4.2*x* and v5.0*x*) are shown in Figure 3.19.2. The profile is shown in both volume mixing ratio (vmr) and density units. All MLS data are reported in vmr for consistency with the other retrieved molecules. However, use of density units (10^6 cm^{-3}) reduces the apparent steep gradient of OH vertical profile, allowing one to see the profile with more detail, especially in the stratosphere where most atmospheric OH is present. Additionally, at THz frequencies the collisional line-width is approximately equal to the Doppler width at 1 hPa. Above 1 hPa, Doppler broadening is dominant and the peak intensity of OH spectral absorption is proportional to density, while below 1 hPa the peak intensity is proportional to vmr. The daytime OH density profile shows two peaks at ∼45 km and ∼75 km. The night OH profile exhibits the narrow layer at ∼82 km [*Pickett et al.*, 2006a]. Precisions are such that an OH zonal average within a 10° latitude bin can be determined with better than 10% relative precision with one day of data (∼100 samples) over 21–0.01 hPa. With 4 days of data, the 10% precision limits can be extended to 32–0.0046 hPa.

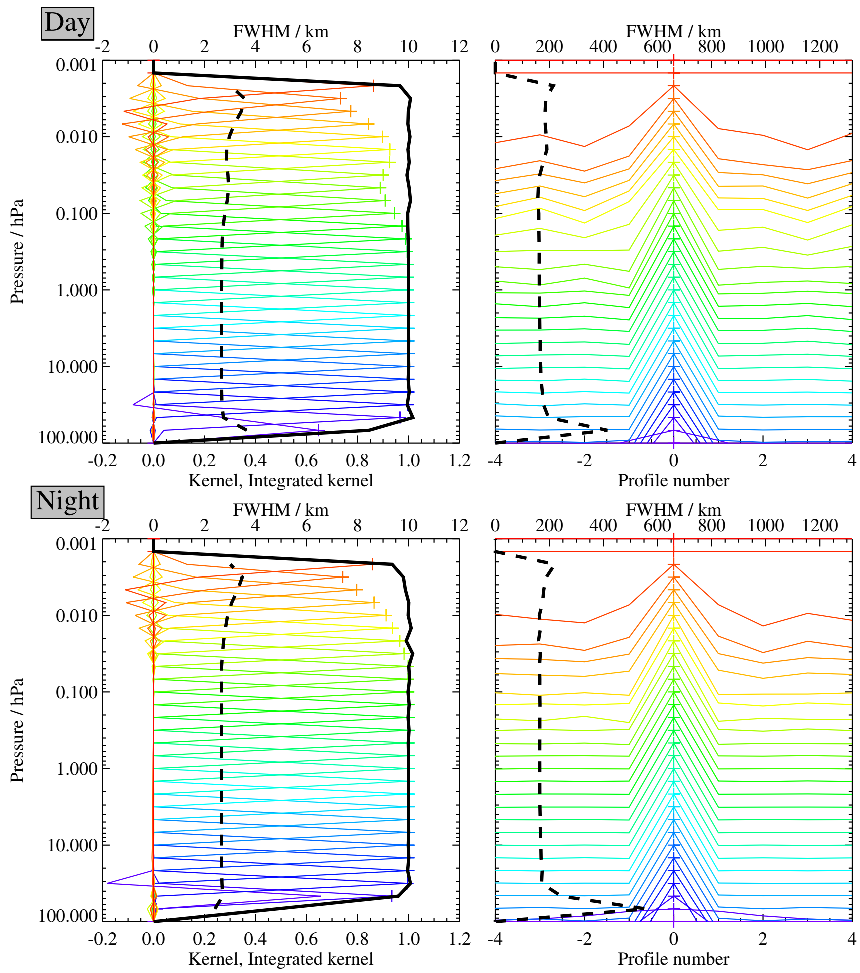

Figure 3.19.1: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x OH data at 35°N for daytime (upper) and nighttime (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The averaging kernels are scaled such that a unit change is equivalent to one decade in pressure.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

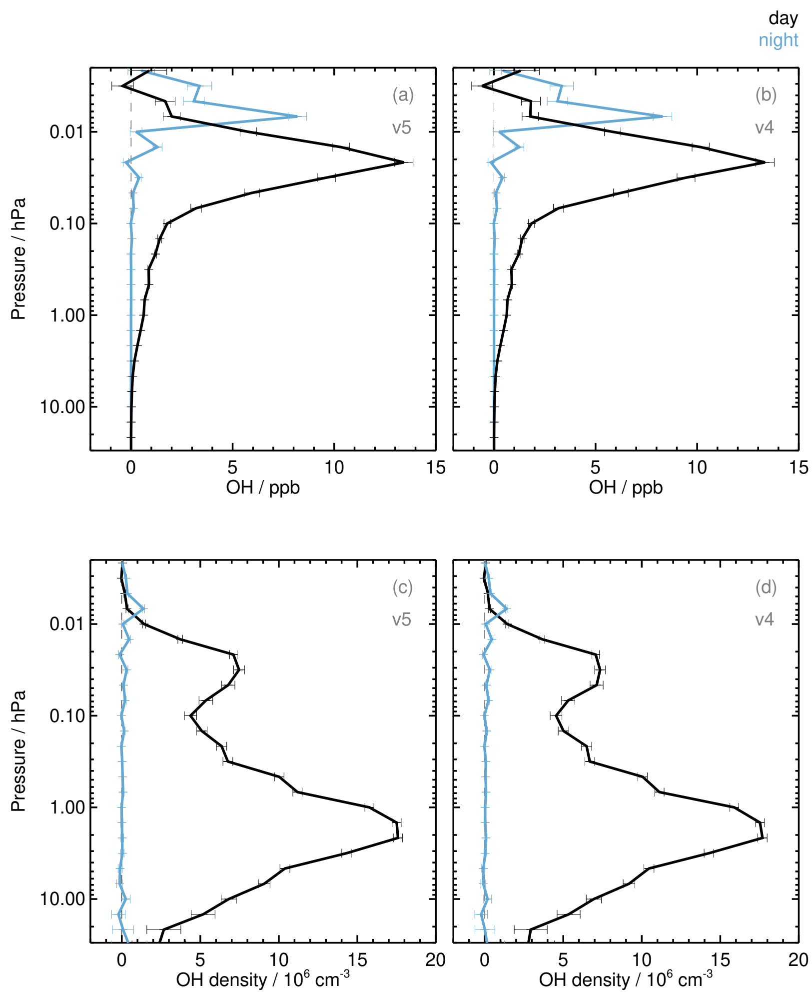

Figure 3.19.2: Zonal mean of retrieved OH and its estimated precision (horizontal error bars) for October 1, 2009 averaged over 29°N to 39°N. The average includes ~100 profiles. Panel (a) shows v5.0x OH vmr vs. pressure for day (black) and night (blue). The retrieved night OH concentration is near zero for altitudes below 1 hPa. Note that the day-night difference is required for altitudes below 10 hPa. Panel (c) shows the same data in (a) converted into density units. Panels (b) and (d) are equivalent to (a) and (c) but using v4.2x OH data.

3.19.4 Accuracy

Table 3.19.1 summarizes the accuracy expected for OH. The effect of each identified source of systematic error on MLS measurements of radiance has been quantified and modeled [*Read et al.*, 2007]. These quantified effects correspond to either 2σ estimates of uncertainties in each MLS product, or an estimate of the maximum reasonable uncertainty based on instrument knowledge and/or design requirements. Biases can be eliminated by taking day-night differences from 32–15 hPa. For 10–0.1 hPa, the observed night OH concentration is small and day-night differencing is not ordinarily needed. The overall uncertainty is the square root of the sum of squares of the precision and accuracy.

3.19.5 Data screening

It is recommended that OH data values be used in scientific investigations if all the following tests are successful:

Pressure range: 32–0.0032 hPa.

Values outside this range are not recommended for scientific use.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality: MLS v5.0*x* OH data can be used irrespective of the value of the `Quality` field.

Convergence: Only profiles whose `Convergence` field is less than 1.1 should be used.

3.19.6 Artifacts

For some seasons, the Gas Laser Local Oscillator (GLLO) for the THz receiver is automatically “relocked” as many as 5 times during a day, leading to data gaps. In these cases the `Status` flag is set to `257` and the profile is ignored. This can present a problem when compiling maps, because the missing data may appear at the same latitude and longitude on successive days.

3.19.7 Review of comparisons with other datasets

Data from MLS v2.2 software have been validated with two balloon-borne remote-sensing instruments and with ground-based column measurements. Details of the comparison are given in *Pickett et al.* [2008] and *Wang et al.* [2008]. The comparison among v2.2 and v5.0*x* show no significant differences except for the mesosphere where v5.0*x* OH daytime values are somewhat larger and less noisy in the summer hemisphere (or tropics when near equinox).

Table 3.19.1: Summary of precisions, resolution, and uncertainties for the MLS OH product

Pressure	Resolution V × H /km	Precision[a] (day/night) / 10^6 cm^{-3}	Accuracy / 10^6 cm^{-3}	Comments
<0.003 hPa	—	—	—	Unsuitable for scientific use
0.003 hPa	5.0 × 220	0.4 / 0.4	0.5	
0.01 hPa	2.5 × 180	1.0 / 0.7	2	
0.1 hPa	2.5 × 165	3.6 / 0.5	1.0	
1.0 hPa	2.5 × 165	2.8 / 0.6	1.0	
10 hPa	2.5 × 165	4.7 / 2.8	1.0	
32–14 hPa	2.5 × 165	13.7 / 12.2	1.5[b]	
>32 hPa	—	—	—	Unsuitable for scientific use

[a]Precision on an individual profile
[b]Use day–night difference

3.20 Relative Humidity with respect to Ice (RHI)

Swath name: RHI

Useful range: UTRHI, mean layer value for P ≤ 383 hPa, Profile from 316–0.001 hPa.

Contact: William Read, **Email:** <william.g.read@jpl.nasa.gov>

3.20.1 Introduction

The vertical grid for the relative humidity with respect to ice (RHI) product is 12 levels per decade change in pressure for 1000–1.0 hPa thinning to 6 levels per decade for 1.0–0.1 hPa and finally 3 levels per decade for 0.1–10^{-5} hPa. The RHI product is a fusion of results from two separate retrievals. From 1000–383 hPa, RHI is retrieved directly from optically thick radiances using measurement and retrieval principles similar to nadir sounding humidity receivers (e.g., TOVS). All grid levels between 1000–383 hPa are filled with a uniform “UTRHI” (upper tropospheric relative humidity with respect to ice) value representing the mean value of a broad layer (∼4–6 km) that peaks between ∼350 hPa (in the moist tropics) and ∼650 hPa (typical for dry high latitudes). This humidity is used as a lower altitude constraint and *a priori* for the vertically resolved humidity product that begins at 316 hPa. From 316–10^{-5} hPa, RHI is derived from the standard products of water and temperature using the Goff-Gratch ice humidity saturation formula. RHI validation is presented in *Read et al.* [2007]. Table 3.20.1 is a summary of precision, resolution, and accuracy. The accuracy figures for v5.0*x* have yet to be determined but are not expected to differ significantly from those of v4.2*x*, the source of the values listed here.

3.20.2 Changes from v4.2*x*

There are no changes between v5.0*x* and v4.2*x* for the UTRHI (1000–383 hPa) retrieval approach. RHI for pressures ≤ 316 hPa is a derived product from H_2O and Temperature and reflect changes in H_2O (3.9) and temperature (3.22).

Figure 3.20.1 compares MLS v5.0, v4.2, and v3.3 to v2.2. The changes seen in here mostly reflect those seen for H_2O because H_2O experienced bigger changes than temperature in this version.

Relative humidity data at pressures greater than 316 hPa are derived from a broad layer relative humidity retrieval (using low limb viewing MLS wing channel radiances) similar to that obtained from NOAA operational humidity sounders such as TOVS. As noted in [*Read et al.*, 2007], the v2.2 retrieval at these pressures was likely to be ∼30% too high based on comparisons with AIRS. The accuracy of this retrieval is highly sensitive to the transmission efficiency of the MLS optics system. In v3.3 this was adjusted empirically (within the uncertainty range established from MLS calibration) to give better agreement with AIRS in the tropics. In v4 the N_2 continuum was adjusted only for this phase to minimize the clear sky cloud induced radiance bias. Other than changes to sideband fractions and pointing offsets detailed in section 3.9, no specific changes are implemented for v5.0*x*. This retrieval is used as an a priori and profile constraint for the humidity profile at pressures greater than 316 hPa which are not retrieved in the standard H_2O product retrieval.

The third panel in Figure 3.20.1 shows the mean estimated single profile precision and the measured variability (which includes instrument noise and atmospheric variability). The precisions among the versions are similar and in the lower stratosphere and upper troposphere are much less than the measured atmospheric variability. The precision for 383 hPa (and higher pressures) is reported in the `L2GP` as 0% by mistake. The actual precision is typically 0.2%.

3.20.3 Resolution

RHI for pressures of 316 hPa and smaller is a derived product and therefore a retrieval averaging kernel is not directly available. An estimate for the spatial resolution (vertical ×along track) of this product is a

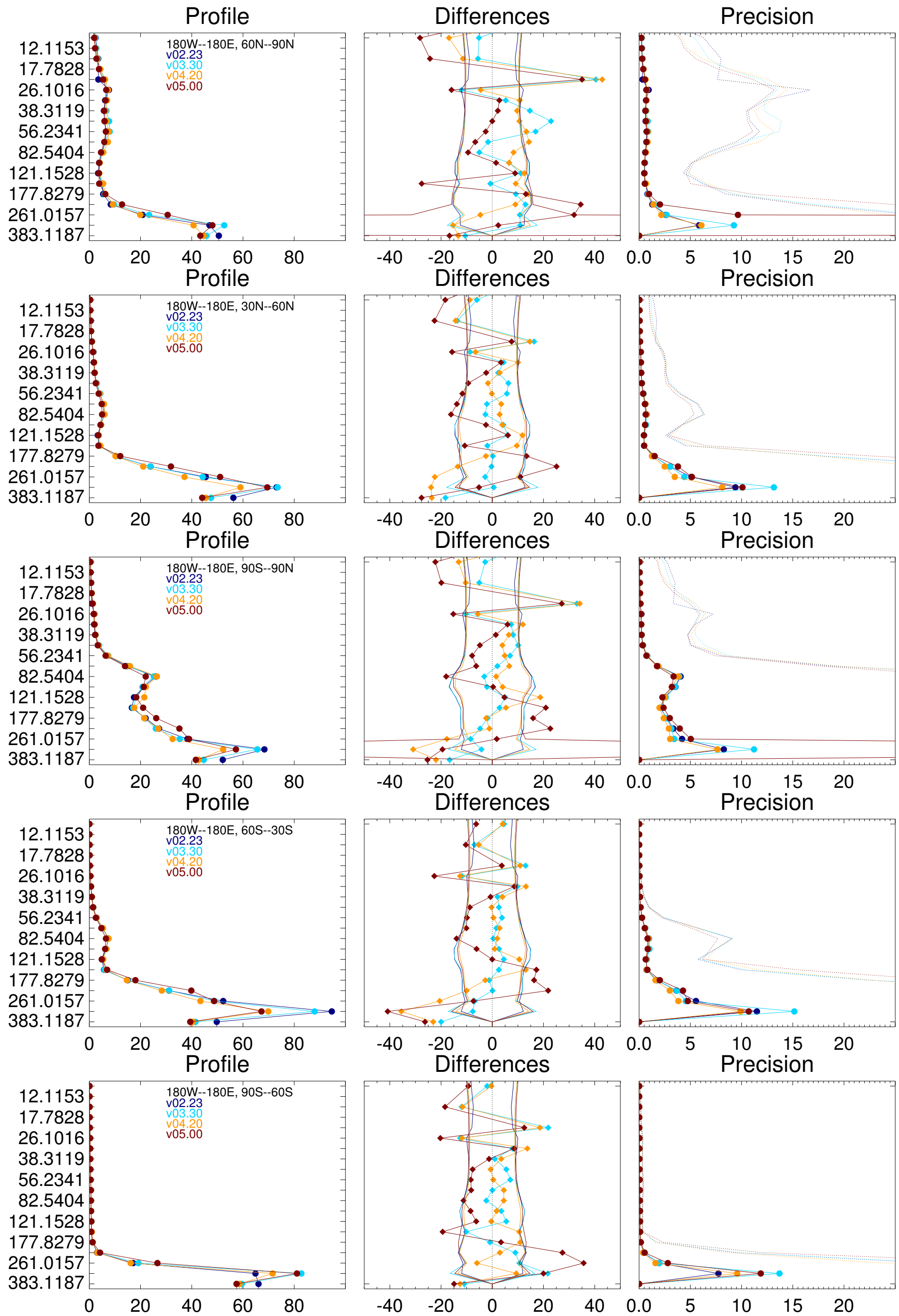

Figure 3.20.1: A zonal mean comparison of RHI profiles in 5 latitude bands. v2.2 (blue), v3.3 (cyan), v4.2 (orange), and v5.0 (red) RHI for Jan-Feb-Mar 2009. Other time periods are similar. The left panel shows the mean profiles, the center shows the mean difference from v2.2 (cyan, orange and red lines with diamonds). The colored lines without symbols are each versions' estimated precision. The right panel shows the estimated retrieval precision (solid lines with bullets) and measured variability (dotted lines) which includes atmospheric variability about the mean profile. X-axes are RHi in percent, y-axis are pressure in hPa.

convolution of the temperature and H_2O resolutions. Typically H_2O has the poorer horizontal resolution and temperature has the poorer vertical resolution. Therefore for estimating spatial resolution, the horizontal resolution is from H_2O and the vertical resolution is from temperature (see 3.9 and 3.22). The cross track resolution is probably 12 km, the larger of temperature and H_2O cross track resolutions. These resolutions are only true in the limit that the mean $\log(H_2O)$ doesn't change appreciably over the broader temperature measurement volume. The longitudinal separation of the MLS measurements, set by the Aura orbit, is 10°– 20° over middle and lower latitudes, with much finer sampling in polar regions.

The RHI for pressures greater than 316 hPa, represents a mean value in a broad layer (4–6 km) whose sensitivity peaks between ∼350 hPa (in the moist tropics) and ∼650 hPa (typical for dry high latitudes).

3.20.4 Precision

The values for precision are the root sum square (RSS) precisions for H_2O and temperature propagated through the Goff-Gratch relationship, see sections 3.9 and 3.22 for more details. The precisions are set to negative values (or zero in some cases) in situations when the retrieved precision is larger than 50% of the a priori precision for either temperature or H_2O — an indication that the data is biased toward the a priori value. The precisions for levels between 1000 and 383 hPa (vertical levels 1–6) are reported as 0% by error. It should typically be 0.2% and is one value for all levels between 1000 and 383 hPa.

3.20.5 Accuracy

The values for accuracy are the RSS accuracies for H_2O and temperature scaled into % RHI units. see sections 3.9 and 3.22 for more details.

3.20.6 Data screening

Pressure range: Profile from 316–0.001 hPa, larger pressures represent mid/upper troposphere column.

Values outside this range are not recommended for scientific use.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Clouds: Ignore status bits 16 (high clouds) or 32 (low clouds) set indicating the presence of clouds. See artifacts for more details.

Quality field: The `Quality` fields for both the `L2GP-RHI` and `L2GP-Temperature` swaths need to be considered, as described below:

For pressures of 83 hPa and smaller: Use only profiles with RHI `Quality` *greater* than 0.7 and Temperature `Quality` *greater* than 0.2

For pressures of 100 hPa and larger: Use only profiles with RHI `Quality` *greater* than 0.7 and Temperature `Quality` *greater* than 0.9.

Convergence field: Only profiles with a value of the RHI `Convergence` *less* than 2.0 and Temperature `Convergence` *less* than 1.03 should be used in scientific studies.

Help Overview Table BrO CH3Cl CH3CN CH3OH ClO CO GPH H2O HCl HCN HNO3 HO2 HOCl IWC IWP N2O O3 OH RHI SO2 T Lvl 3

Temperature precision: The `L2gpPrecision` field in the `L2GP-Temperature` file can be used to further eliminate outliers that are believed to be the result of thick clouds, primarily in the tropics. If careful screening of the troposphere is required, levels 261–178 hPa should be avoided if any of the following criteria are met:

At 316 hPa: `L2gpPrecision` > 1.1 K **and** latitude $> -60°$

At 261 hPa: `L2gpPrecision` > 0.7 K

At 215 hPa: `L2gpPrecision` > 0.825 K

Additional screening for based on H_2O: Eliminate highly oscillatory profiles by eliminating H_2O profiles having values less than 0.101 ppmv at any pressure < 1 hPa (vertical levels 1–37).

3.20.7 Artifacts

See sections 3.9 for H_2O and 3.22 for temperature for specific issues related to these parent products. Effects of MLS temperature precision ($\sim$1–2 K) must be considered if one wishes to use MLS RHI to study supersaturation. In simulation studies, systematic errors (such as tangent pressure retrieval and errors), in addition to introducing biases, also increase variability in differences with respect to a "truth" data set particularly for pressures greater than 200 hPa. This will add to the frequency of supersaturation in the tail of MLS RHI distribution functions. Therefore, MLS RHI is not recommended for studying statistics of supersaturation at pressures greater than 178 hPa. For smaller pressures, one must remove the contribution from temperature noise as part of the analysis. Measurements taken in the presence of clouds significantly degrade the precision, that is increases the scatter about the mean, but the mean bias as compared to AIRS changes by less than 10%.

Also, users should note the possibility of a potential drift in the MLS lower stratospheric water vapor product, discussed in section 3.9.8. Such a drift will also impact the RHI product.

3.20.8 Review of comparisons with other datasets

Figures 3.20.2 and 3.20.3 show comparisons between AIRS v6 and MLS v2.2, v3.3, v4.2 and v5.0. Mapped features tend to agree well but MLS produces higher relative humidities in the moist regions of the tropics relative to AIRS. Except as noted previously, the four MLS versions show little change amongst themselves.

3.20.9 Desired improvements

While many defects in v4.2 and earlier versions have been addressed, further investigation into their effectiveness, especially the drift reduction and high latitude low value retrievals in the upper troposphere needs to be assessed and improved upon if necessary. Retrieval of vertically resolved H_2O for pressures > 316 hPa may be possible at high latitudes during dry conditions, but that remains to be investigated.

Help Overview Table BrO CH3Cl CH3CN CH3OH ClO CO GPH H2O HCl HCN HNO3 HO2 HOCl IWC IWP N2O O3 OH RHI SO2 T Lvl 3

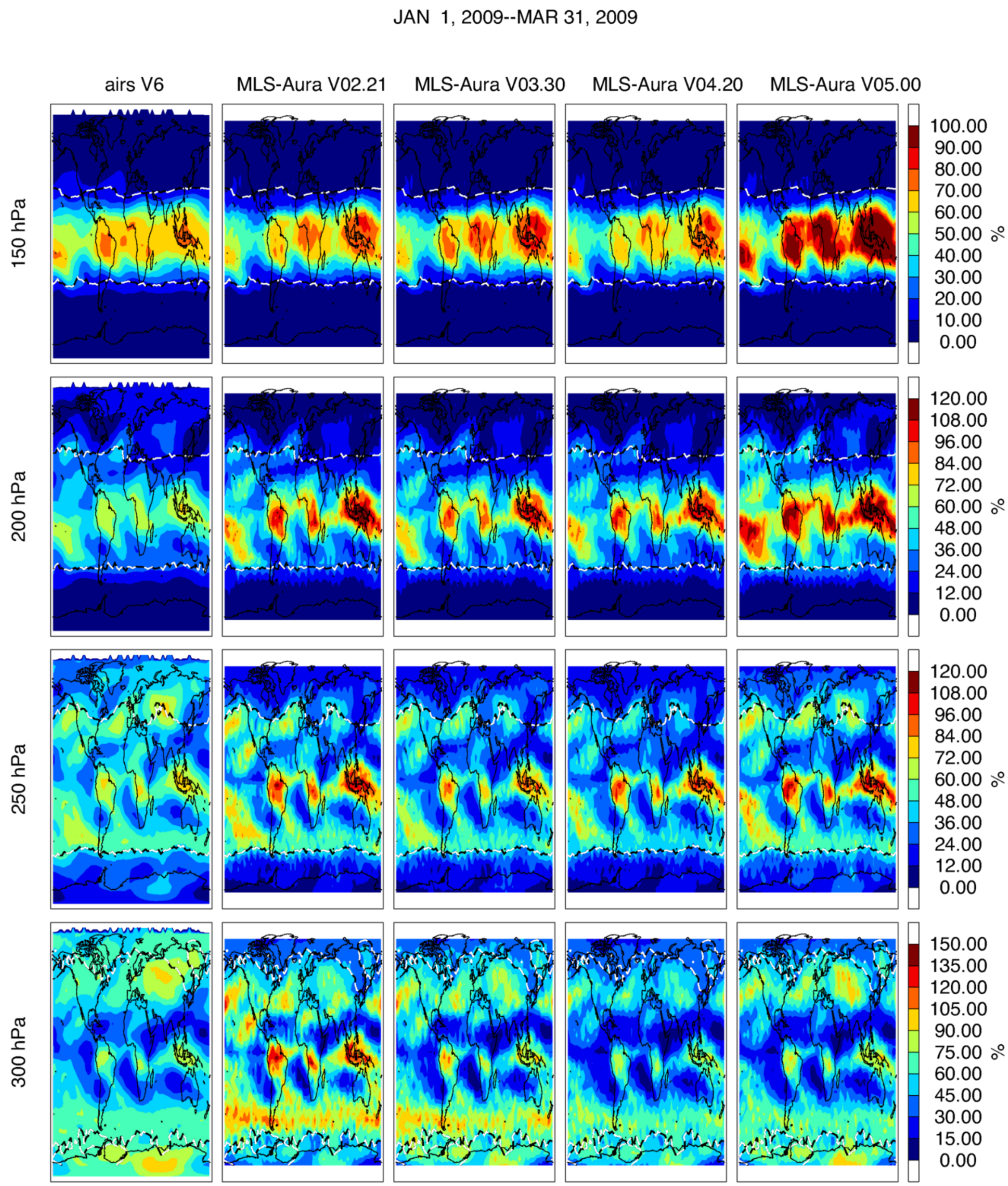

Figure 3.20.2: Mapped fields from AIRS v6 (left panel), MLS v2.2 (2nd from left), MLS v3.3 (3rd from left), MLS v4.2 (4th from left) and MLS v5.0 (right panel) pressures between 300–150 hPa for January, February, and March 2009. The black-white lines indicate the tropopause where the region poleward is in the stratosphere.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

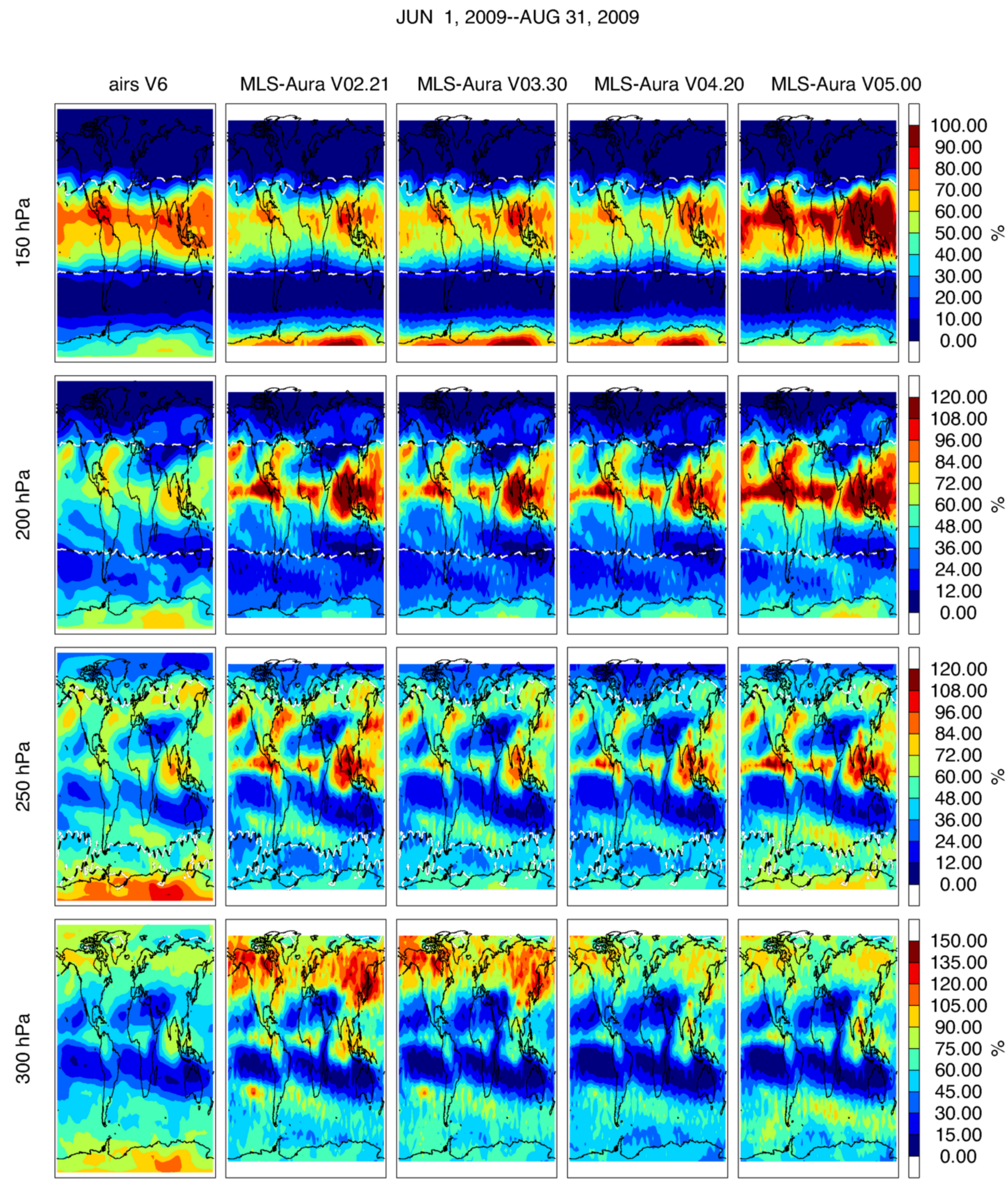

Figure 3.20.3: Mapped fields from AIRS v6 (left panel), MLS v2.2 (2nd from left), MLS v3.3 (3rd from left), MLS v4.2 (4th from left) and MLS v5.0 (right panel) pressures between 300–150 hPa for June, July, and August 2009. The black-white lines indicate the tropopause where the region poleward is in the stratosphere.

Help
Overview
Table
BrO S T
CH_3Cl S T
CH_3CN S T
CH_3OH S T
ClO S T
CO S T
GPH S T
H_2O S T
HCl S T
HCN S T
HNO_3 S T
HO_2 S T
HOCl S T
IWC S T
IWP S T
N_2O S T
O_3 S T
OH S T
RHI S T
SO_2 S T
T S T
Lvl 3

Table 3.20.1: Summary of MLS v5.0x UTLS RHI product.

Pressure / hPa	Resolution V × H km	Single profile precision [a] / %	Accuracy[b] / %	Comments
0.00046	—	—	—	Unsuitable for scientific use
0.001	13.9 × 708	393	59	
0.002	14.0 × 508	157	53	
0.004	14.7 × 428	81	37	
0.010	13.8 × 398	61	31	
0.022	12.0 × 374	50	34	
0.046	10.6 × 318	42	36	
0.10	8.0 × 270	40	35	
0.22	8.2 × 262	28	25	
0.46	8.3 × 261	18	17	
1.00	7.2 × 316	13	10	
2.15	6.9 × 308	10	15	
4.64	6.1 × 295	10	11	
10	5.5 × 291	10	22	
22	5.3 × 275	10	22	
46	5.3 × 267	10	11	
68	5.4 × 248	11	10	
83	5.6 × 248	11	12	
100	5.8 × 251	12	25	
121	5.6 × 259	11	23	
147	5.1 × 259	11	14	
178	5.0 × 263	11	13	
215	4.5 × 263	11	19	see Table 3.9.1
261	4.7 × 253	10	24	see Table 3.9.1
316	4.4 × 253	14	35	see Table 3.9.1
UTRHI, >316	6 × 155	40(est)	10(est)	measurement height depends on atmospheric humidity

[a] Absolute error in percent
[b] Fractional error ([error in RHI] / RHI) in percent

3.21 Sulfur Dioxide (SO_2)

Swath name: SO2

Useful range: 215–10.0 hPa

Contact: William Read, **Email:** <william.g.read@jpl.nasa.gov>

3.21.1 Introduction

The standard SO_2 product is taken from the 240-GHz retrieval (`CorePlusR3`). MLS can only measure significantly enhanced concentrations above nominal background such as that from volcanic injections. Validation of SO_2 is published in *Pumphrey et al.* [2015].

3.21.2 Changes from v4

Changes in the 240-GHz MLS products from v4.2*x* to v5.0*x* are minor and mostly affect O_3 and CO. A new O_3 *a priori* and updated smoothing parameters are incorporated, and a non-linear radiance model is used to calculate the signals in the high spectral resolution digital autocorrellator spectrometer (DACS) channels for the O_3 and CO lines. In addition to these changes, the accuracy threshold for the non-linear radiance model calculations was reduced from 0.02 K to best possible (i.e., 0 K). These changes will have secondary impacts on SO_2.

Figure 3.21.1 compares MLS v4.2 and v3.3. The atmosphere typically has ~0.1 ppbv SO_2, which is far smaller than the MLS SO_2 accuracy estimate. All versions (erroneously) report typical abundance of order of a few ppbv, due to systematic errors in the MLS measurement system. The −20 ppbv reported at 215 hPa is also a systematic artifact. Changes from v2 through to v4 involved handling of the background radiance signals which evolved from an absorption continuum (v2) to an RHi continnuum (v3) to a MLS minor frame absorption continuum with a frequency squared spectral dependence (v4 and v5). Versions 4 and 5 also uses improved cloud detection and radiance screening for them.

3.21.3 Resolution

Based on Figure 3.21.2, the vertical resolution for SO_2 is ~3 km and the horizontal resolution is 170 km. The horizontal resolution perpendicular to the orbit track is 6 km, the full width at half maximum of the MLS antenna, for all pressures.

3.21.4 Precision

The estimated precision for SO_2 is ~4 ppbv for all heights between 215–10 hPa. The precisions are set to negative values (or zero in some cases) in situations when the retrieved precision is larger than 50% of the a priori precision – an indication that the data is biased toward the a priori value. Even though the changes between v4 and v5 are minor, there is a change in the estimated precision. An example of this is shown in Figure 3.21.3. SO_2 precision from v5 shows much less variability and less latitude dependence than v4. Although only 100 hPa is shown here, it is similar for other stratospheric levels and it also affects other species retrieved from the 240-GHz radiances, such as HNO_3. The change in behavior occurred as a result of reducing the forward model accuracy threshold from 0.02 K to "best possible."

3.21.5 Accuracy

Accuracy is estimated to be 10–20 ppbv over the useful pressure range. These are not expeted to change significantly for the v5 SO_2 product yet to be determined.

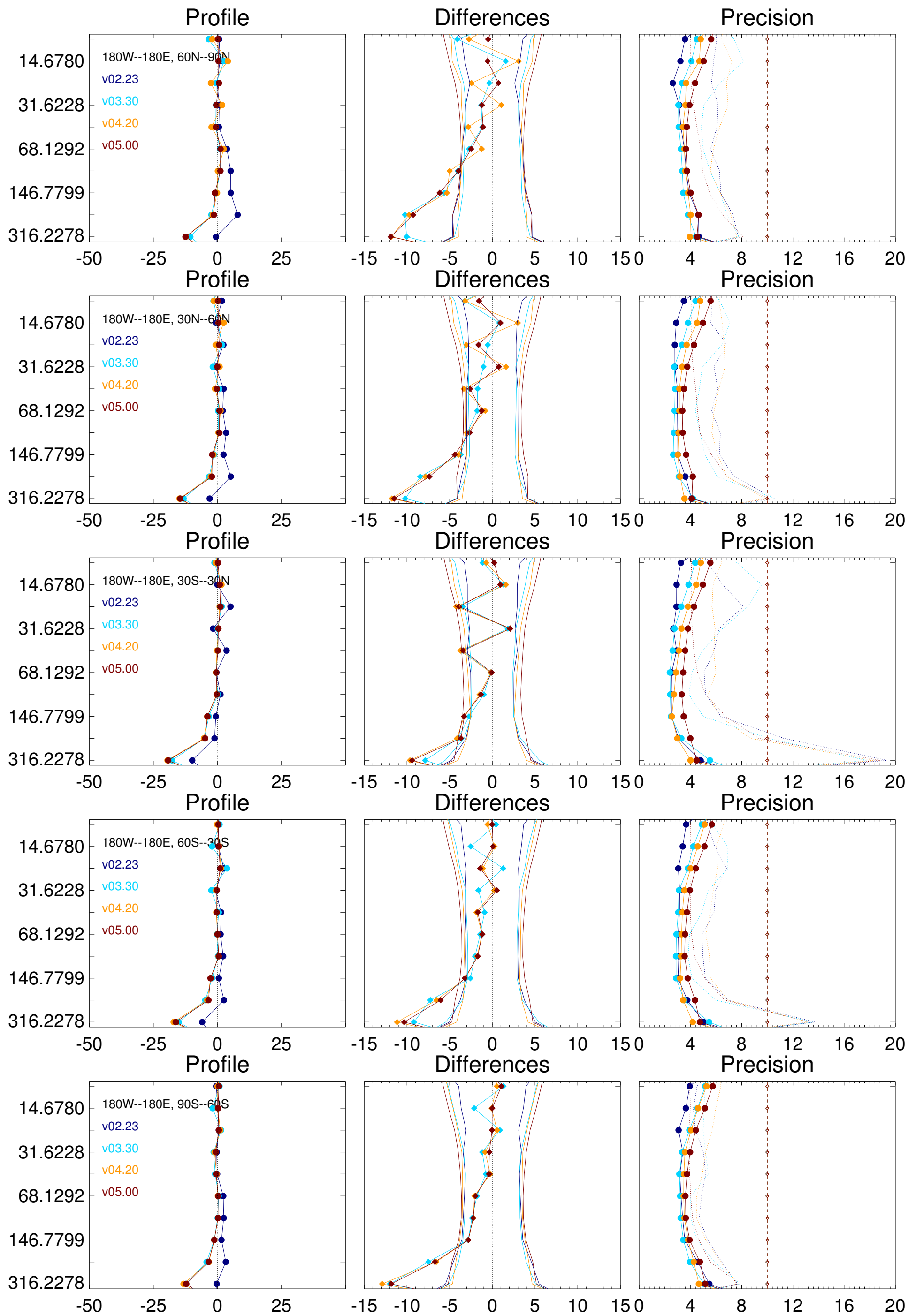

Figure 3.21.1: A comparison of v2.2 (dark blue), v3.3 (light blue), v4.2 (orange) and v5.0 (red) SO_2 for Jan-Feb-Mar 2009 in five latitude bands. Other time periods are similar. The left panel compares mean profiles, the center shows the mean difference (red diamonds) surrounded by each versions' estimated precision, and the right panel shows the estimated retrieval precision (solid and bullets), measured variability (dotted) which includes atmospheric variability about the mean profile, and a priori precision (dashed and diamonds).

Help Overview Table BrO CH$_3$Cl CH$_3$CN CH$_3$OH ClO CO GPH H$_2$O HCl HCN HNO$_3$ HO$_2$ HOCl IWC IWP N$_2$O O$_3$ OH RHI SO$_2$ T Lvl 3

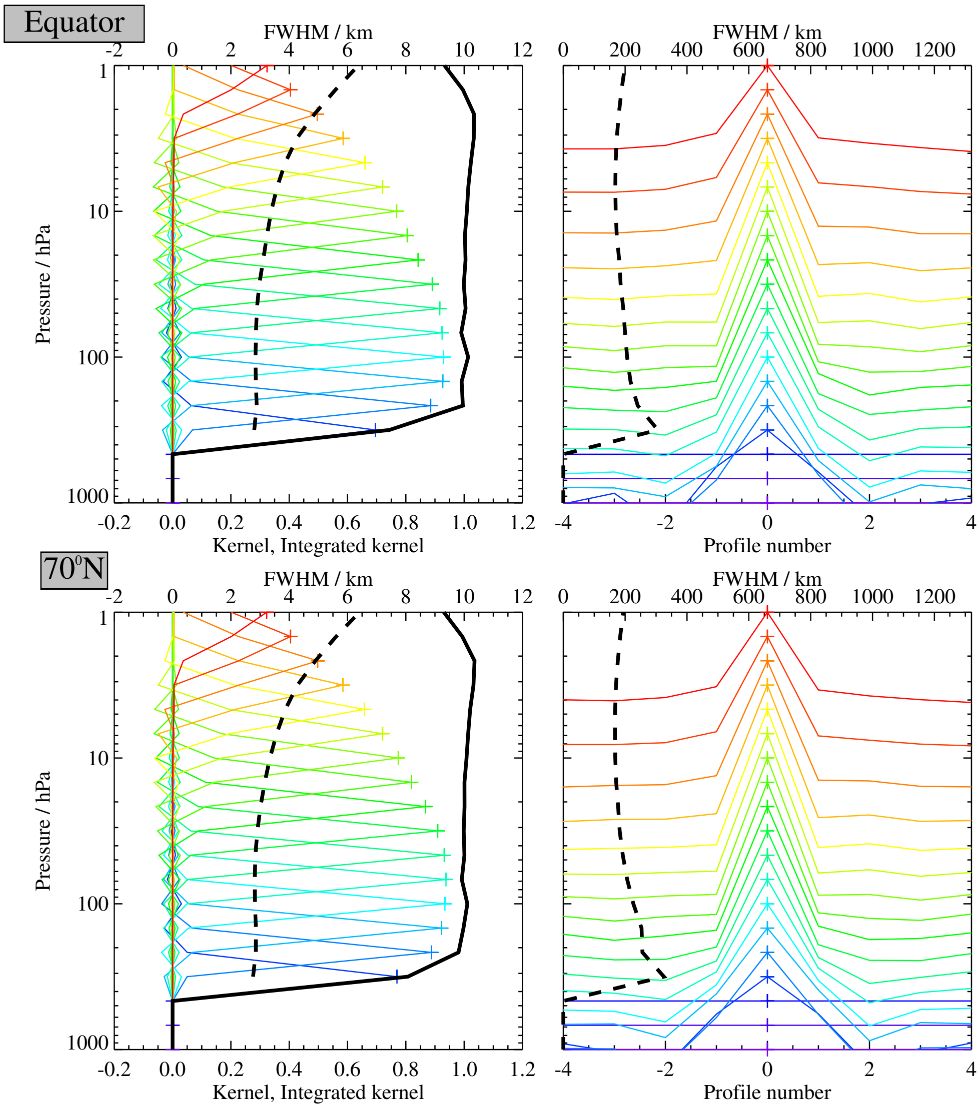

Figure 3.21.2: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x SO_2 data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

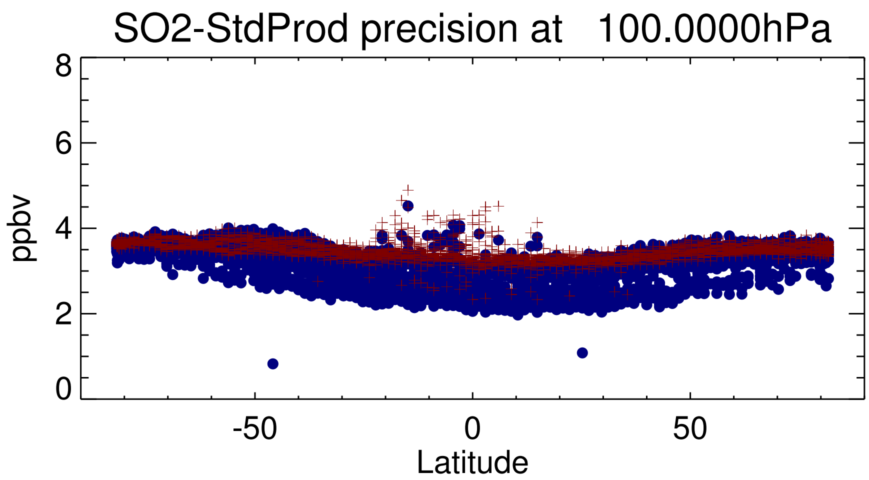

Figure 3.21.3: A comparison of estimated precision for SO_2 from v4 (blue) and v5(red) and 100 hPa.

3.21.6 Data screening

Pressure range: 215–10.0 hPa

Values outside this range are not recommended for scientific use.

Estimated Precision: Values with negative precision can be used, though with caution.

Although it is generally recommended to not use values where precision is flagged negative, SO_2 is an exception and it is appropriate to use values with negatively flagged precision (provided that the entire profile is not so flagged). High retrieved values of SO_2 at the larger pressures (e.g., 215 and 147 hPa) will also have larger (i.e., poorer) precision values which are sometimes large enough to trigger the "too much *a priori* influence" negative-precision flag. In these cases, there will be an *a priori* influence, and the retrieved value will probably be smaller than reality because the retrieval is being pulled towards the *a priori* value of zero ppbv. Nonetheless, this does not detract from the fact that greatly enhanced SO_2 is being observed, reflecting the detection of a plume. Profiles where the precision is set to zero, however, should be omitted from analyses.

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality field: Only profiles having `Quality` *greater* than 0.95 should be used.

As with water vapor, this value represents where the quality versus yield sharply drops indicating the transition from well fit profiles toward more poorly fit ones as shown in Figure 3.21.4

Convergence field: Only profiles having `Convergence` *less* than 1.03 should be used.

3.21.7 Artifacts

High values of SO_2 accompanied with negative errors are likely to be underestimated due to *a priori* influence which biases the value toward zero. The atmospheric background SO_2 ($\sim$0.1 ppbv) cannot be measured by MLS even with extensive data averaging because there are systematic errors producing biases of a few ppbv. The 215-hPa SO_2 has a background bias of approximately −20 ppbv.

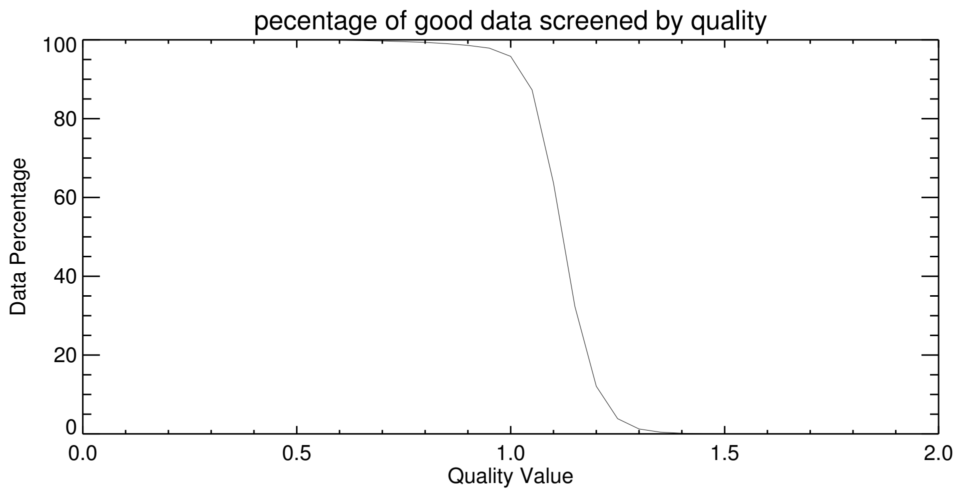

Figure 3.21.4: Percentage of data having a quality greater than that indicated on the x-axis for v5.0 data processed for June-July-August 2005.

3.21.8 Review of comparisons with other datasets

MLS has successfully detected SO_2 from many eruptions since launch.

Figure 3.21.5 shows an overlay comparison of column SO_2 measured by OMI and the same calculated by MLS for two days following the Sarychev eruption. It is clear that MLS detects the main plume dispersal features. It also appears that MLS columns are often smaller than those from OMI. Interpreting the significance of this is not straightforward given that OMI has to make assumptions regarding the profile shape and can observe SO_2 down to the boundary layer. The MLS column begins at 215 hPa and integrates upward neglecting the tropospheric contributions. Another limitation is that OMI can only make measurements during the day whereas MLS can make them day and night. Since the plume is moving relatively quickly over the 12-hour measurement separation time, MLS nighttime measurements often miss and/or detect plume features differently than OMI.

Figure 3.21.6 shows a comparison between v5 and v4 for a track showing the maximum SO_2 measured on 16 June 2009. As expected v5 and v4 show similar amounts of SO_2 at levels 215–68 hPa. Nominally the SO_2 is concentrated between 147 and 100 hPa.

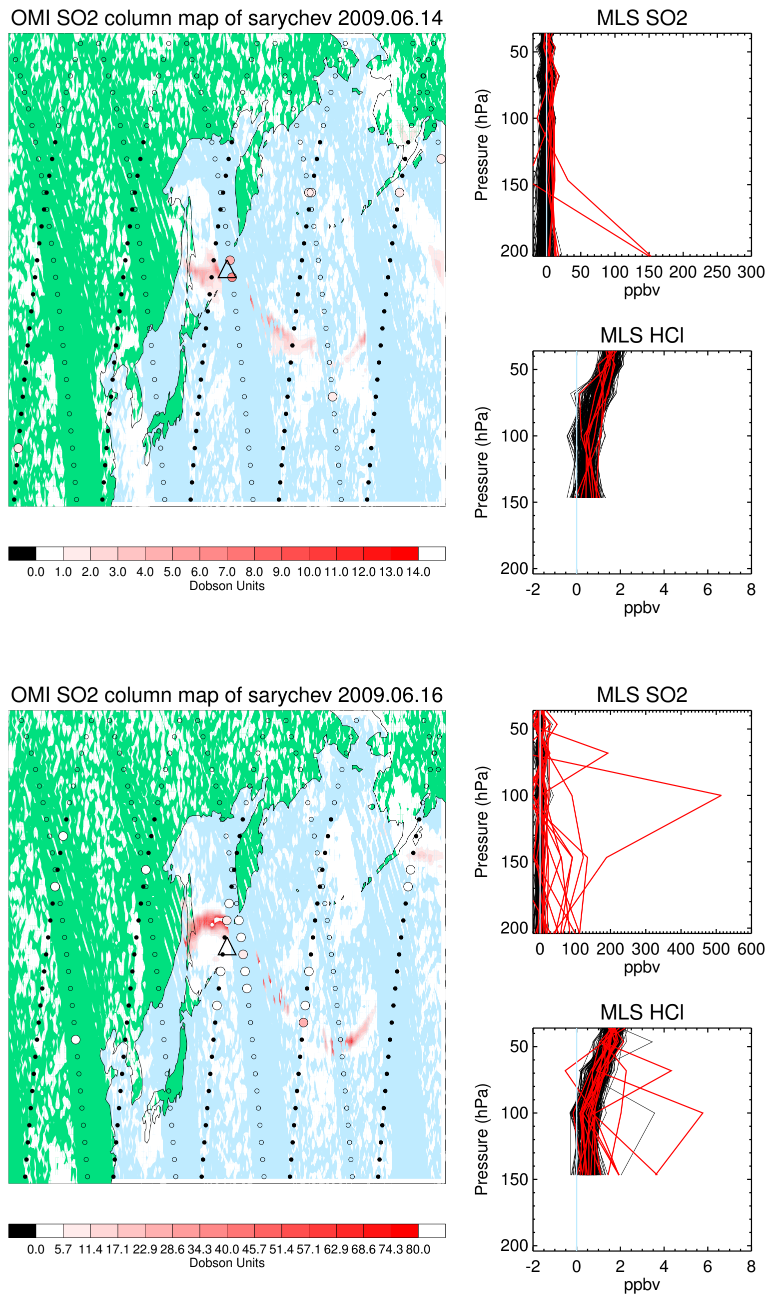

Figure 3.21.5: An overlay of MLS measurement tracks on an OMI SO_2 measurement on 14 and 16 June 2009 (separate maps) showing the dispersial of SO_2 from the Sarychev eruption (13 June 2009, black triangle). The OMI instrument has some non operational pixels also known as the row anomaly where measurements are not possible. It turns out that one of these row anomalies is perfectly aligned with the MLS track and therefore there are no coaligned OMI-MLS measurements. The color scale indicates the SO_2 column measured by OMI. The daytime MLS tracks are small open circles and the nighttime tracks are filled black. When the calculated column from MLS exceeds 1 DU, that measurement is indicated by a larger open circle filled with the color of the column measurement as indicated by the color scale below (same as for OMI). The panels at right show all the measured profiles covering the area shown in the maps for SO_2 and HCl. Profiles where the MLS column calculation exceeds 1 DU are highlighted in red.

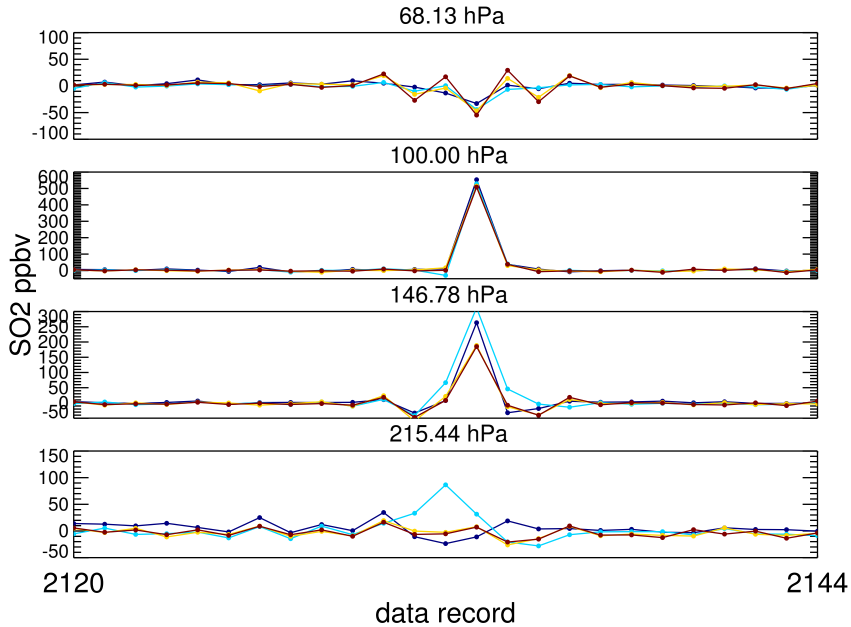

Figure 3.21.6: Time series overlay where MLS measures more than 500 ppbv at 100 hPa for the Sarychev erruption. Blue is version 4, and red is version 5.

Table 3.21.1: Summary of MLS v3.3 SO_2 product.

Pressure / hPa	Resolution V × H km	Single profile precision ppbv	Accuracy / ppbv	Comments
< 10	—	—	—	Unsuitable for scientific use
10	3.6 × 170	5.8	4	
15	3.4 × 170	5.3	4	
22	3.3 × 170	4.5	5	
32	3.0 × 170	4.0	5	
46	3.0 × 170	3.7	4	
68	2.9 × 170	3.6	5	
100	2.9 × 170	3.6	5	
147	2.9 × 170	3.8	10	
215	2.8 × 180	4.4	20	
>215	—	—	—	Unsuitable for scientific use

3.22 Temperature (T)

Swath name: `Temperature`

Useful range: 261–0.00046 hPa

Contact: Michael J. Schwartz, **Email:** <Michael.J.Schwartz@jpl.nasa.gov>

3.22.1 Introduction

The MLS v5.0*x* temperature product is nearly identical to the v4.2*x* product and is generally similar to the v3.3 product and to the v2.2 product that is described in *Schwartz et al.* [2008]. MLS temperature is retrieved primarily from bands near O_2 spectral lines at 118 GHz and 239 GHz that are measured with MLS radiometers R1A/B and R3, respectively. The isotopic 239 GHz line is the primary source of temperature information in the troposphere, while the 118 GHz line is the primary source of temperature in the stratosphere and above. MLS v5.0*x* temperature has an approximately −1 K bias with respect to correlative measurements in the troposphere and stratosphere, with 2–3 K peak-to-peak additional systematic vertical structure. Table 3.22.1 summarizes the measurement precision, resolution, and modeled and observed biases. The following sections provide details.

3.22.2 Differences between v5.0*x* and v4.2*x*

Mean differences between v5.0*x* temperature and v4.2*x* temperature are typically less than 0.2 K, although vertically oscillating bias structure in the tropopause can be as large as ±0.8 K. Temperature v4.2*x* temperature

Both v5.0*x* and v4.2*x* use GEOS-5 "Forward Processing for Instrument Teams" (FP-IT) temperatures as their retrieval *a priori*, each using the version available at the time of processing. v4.2*x* uses GEOS-5.9.1 from the beginning of the mission through 2016 and GEOS-5.12.4 from 2017 into 2020, whereas v5.0*x* uses GEOS-5.12.4 from the beginning of the mission into 2020, and differences in these *a priori* can result in small differences in retrieved values. Throughout the rest of this section, "GEOS-5" without additional qualification refers to GEOS-5.12.4 FP-IT.

Versions v3.x and v2.x took the standard temperature product from `FinalPtan`, a preliminary "phase" of the MLS retrieval that uses only the O_2 bands and that focuses on retrieval of temperature and tangent-point pressure. The standard v5.0*x* and v4.2*x* temperature products are both taken from the `CorePlusR3` phase, which adds radiances from the 240-GHz radiometer and which simultaneously retrieves standard products for a number of atmospheric constituents. The `CorePlusR3` temperature and GPH along with the accompanying tangent-point pressures, are used for all subsequent constituent retrievals, so they are more internally consistent with the suite of constituent retrievals than were the standard temperature and GPH products of previous versions.

MLS is generally insensitive to the presence of thin clouds, but scattering in the cores of convective storms can produce significant perturbations in MLS retrieved quantities, including temperature. Indeed, *a priori* knowledge of temperature from analysis is often so good in the lower and middle atmosphere that perturbations of a few percent (a level typically considered to be negligible for trace-gas constituent retrievals) are considered "significant" for temperature. In the troposphere where *a priori* knowledge may be on the order of 1–2 K, temperatures from an analysis like GEOS-5 (the retrieval *a priori*) may be more reliable than the MLS retrieval product, and differences between the MLS and GEOS-5 temperatures can be useful in the identification of retrieval artifacts. Cloud-induced perturbations generally occur in the tropics and mid-latitudes (where convective storms occur) in both the v5.0*x* and v4.2*x* retrieval versions. In unscreened data at retrieval levels 316–178 hPa, clouds produce primarily positive outliers in v5.0*x* and v4.2*x*. The top panels of Figure 3.22.2 show this behavior at 215 hPa. Conversely, at 121 hPa, outliers are primarily positive in v5.0*x* and v4.2*x*.

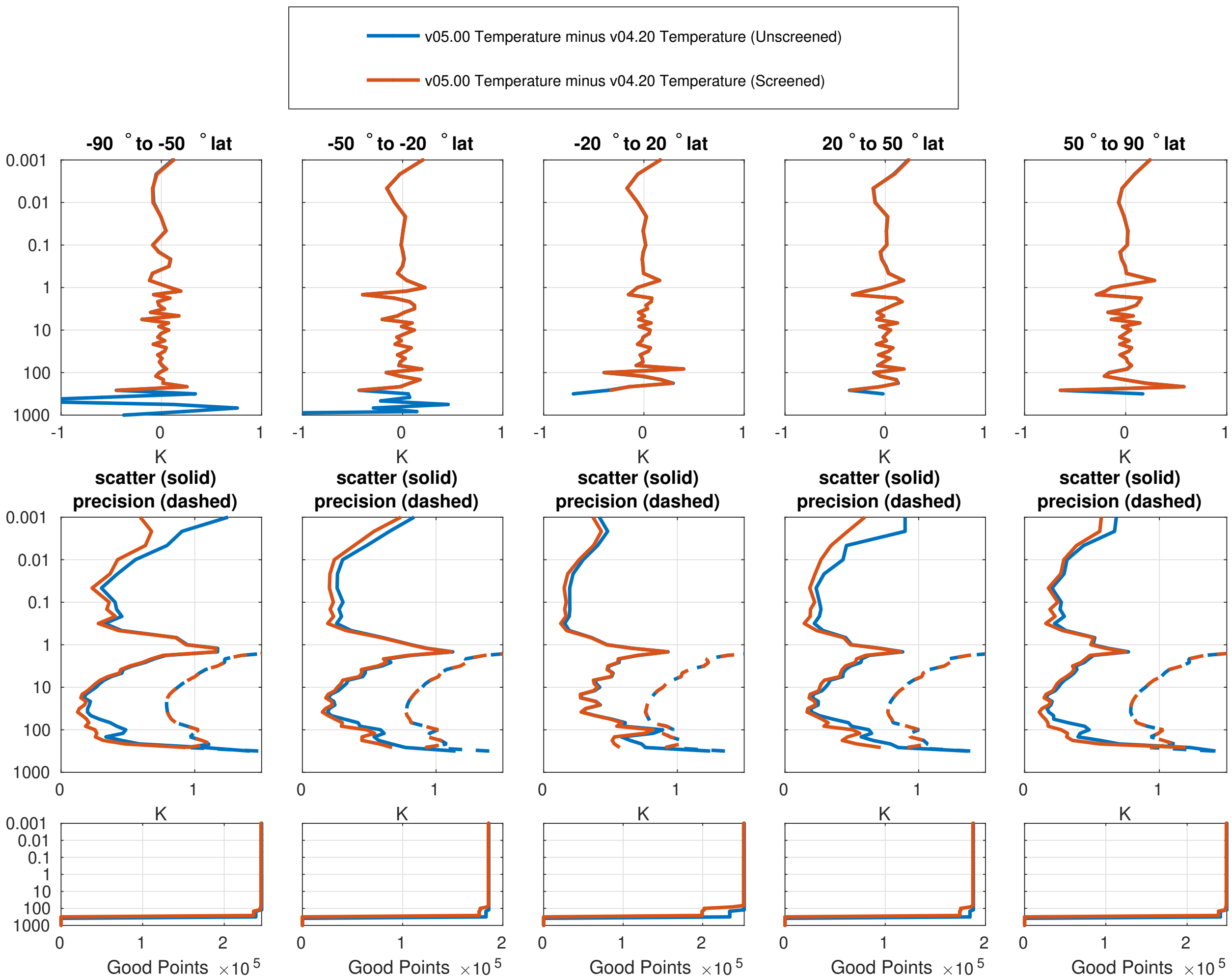

Figure 3.22.1: Temperature differences between v5.0x and v4.2x standard products, screened per recommendations of this document (green) and unscreened (red). 2009 data are shown. Top row is mean difference between versions, binned by latitude. Screening has a significant impact on mean values only at low latitudes in the troposphere. The middle row of panels shows that there is considerably more scatter in unscreened data at the bottom of the retrieval, particularly at low latitudes. The bottom row's difference between red and green lines is the number of points that are screened out. Y-axes are pressure in hPa.

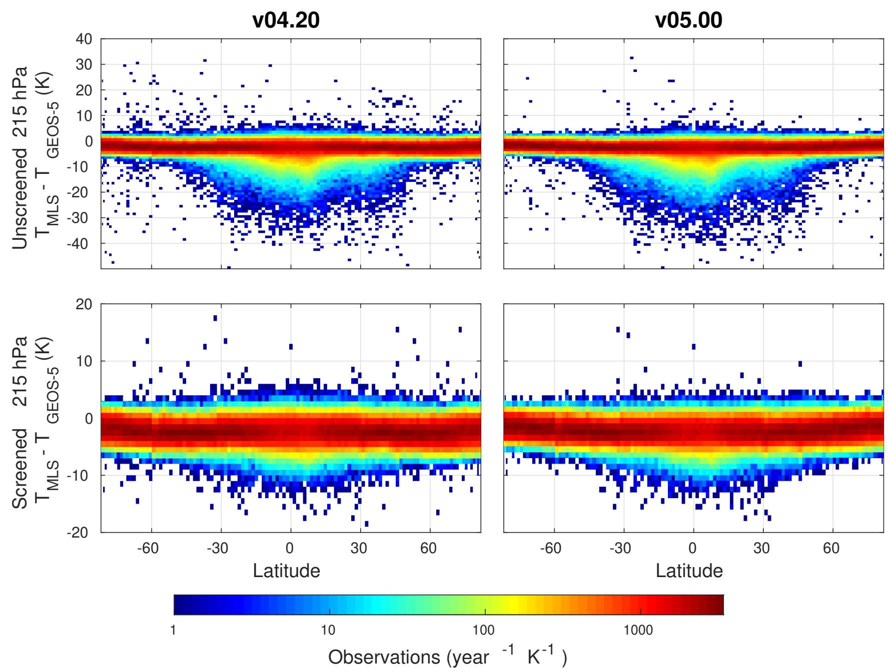

Figure 3.22.2: The top row shows histograms of unscreened 215 hPa v04.20 (left) and v05.00 (right) temperature differences from GEOS-5.9.1 temperature for 2009. The horizontal bin spacing is that of the ~1.5° latitudinal spacing of the MLS scans. The bottom panels show histograms of differences of the screened profiles on a finer vertical scale. Outliers beyond ±20 K have been almost completely eliminated and are not shown.

Unscreened and screened histograms of tropical (20°S–20°N) v5.0*x* and v4.2*x* temperature from 2009 are shown in Figure 3.22.3. Tails of low, unscreened outliers are particularly evident from 316–147 hPa, but are greatly reduced by recommended screening (magenta).

The highest level (lowest pressure) of the v4.2*x* temperature retrieval recommended for scientific work in the previous version of this document is 0.001 hPa, but temperature is retrieved, in both v4.2*x* and v5.0*x*, up to the 0.0001 hPa level. The 0.00046 hPa level is typically near the top tangent point of the MLS scan while the 0.00022 hPa surface is often above the height of the highest tangent point in the MLS limb scan (depending upon latitude). The estimated precision of the retrieval at both of these levels is less than half of the precision of the retrieval *a priori*. However, as can be seen from Figure 3.22.4 for both latitudes shown, the averaging kernels of the 0.00046 hPa retrieval level is sharply peaked at 0.00046 hPa, while the averaging kernel of the 0.00022 hPa retrieval level shows a larger contribution from 0.00046 hPa than from 0.00022 hPa. As was the case in v4.2*x*, the precisions of the 0.00046 hPa and 0.00022 hPa levels in v5.0*x* are set negative “by hand” to advise against their casual use, but for v5.0*x*, we are recommending that 0.00046 hPa temperature may be generally useful, while 0.00022 hPa may have some value in for some scientific studies. Further validation of v5.0*x* temperature at these levels is planned.

3.22.3 Resolution

The vertical and horizontal resolution of the MLS temperature measurement is shown by averaging kernels in Figure 3.22.4 and summarized in Table 3.22.1. Vertical resolution, shown on the left panel, is 3–4 km from 261 hPa to 10 hPa, degrades to 7–8 km at 1–0.1 hPa, and to 11 km at 0.01 hPa, and to 12 km at 0.0001–0.0002 hPa. Along track resolution is ~165 km from 261 hPa to 0.1 hPa and degrades to 280 km at 0.001 hPa and to 316 km at 0.00046 hPa. The cross-track resolution is set by the 6 km width of the MLS 240 GHz field of view in the troposphere and by the 12 km width of the MLS 118 GHz

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

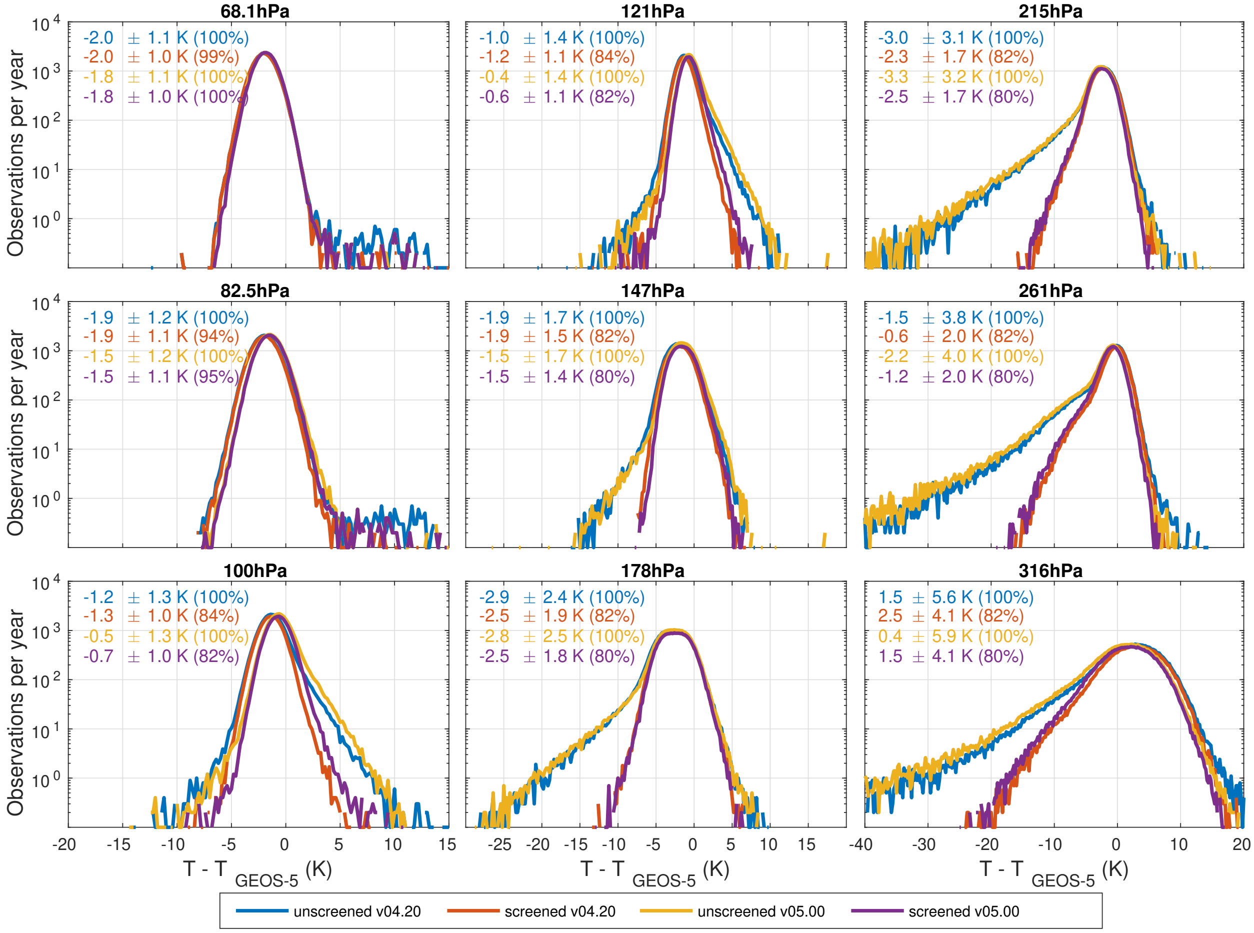

Figure 3.22.3: Panels show histograms of tropical (20°S–20°N) differences between MLS retrieved temperatures and GEOS-5.12.4, temperature for all of 2005. Blue and green lines are unscreened and screened v04.2x, respectively. Red and magenta are unscreened and screened v05.00, respectively. Distribution means and standard deviations are given in the upper left of each panel along with the percentage of points included after screening. The 316-hPa level is shown for reference although this level is not recommended to be used for scientific work.

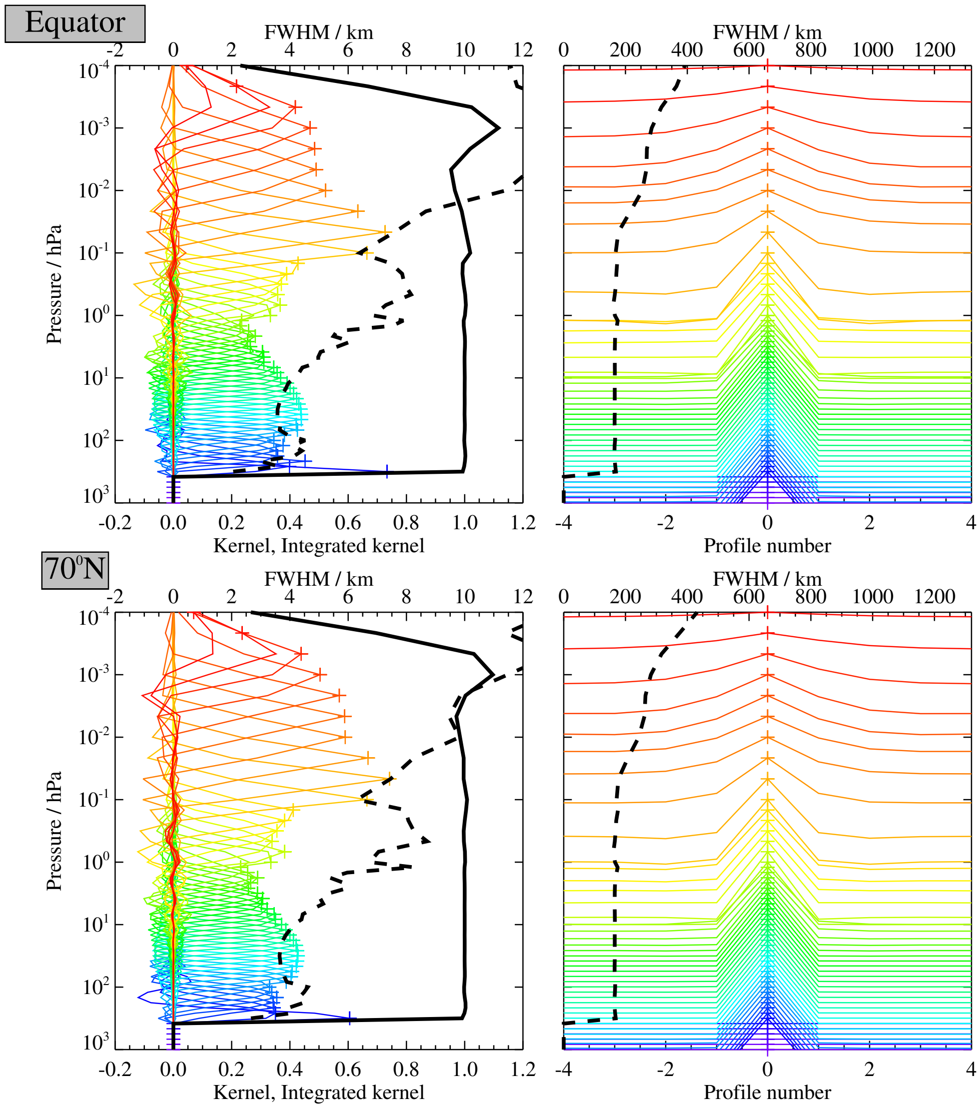

Figure 3.22.4: Typical two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS v5.0x Temperature data at the equator (upper) and at 70°N (lower); variation in the averaging kernels is sufficiently small that these are representative of typical profiles. Colored lines show the averaging kernels as a function of MLS retrieval level, indicating the region of the atmosphere from which information is contributing to the measurements on the individual retrieval surfaces, which are denoted by plus signs in corresponding colors. The dashed black line indicates the resolution, determined from the full width at half maximum (FWHM) of the averaging kernels, approximately scaled into kilometers (top axes). (Left) Vertical averaging kernels (integrated in the horizontal dimension for five along-track profiles) and resolution. The solid black line shows the integrated area under each kernel (horizontally and vertically); values near unity imply that the majority of information for that MLS data point has come from the measurements, whereas lower values imply substantial contributions from a priori information. (Right) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The horizontal averaging kernels are shown scaled such that a unit averaging kernel amplitude is equivalent to a factor of 10 change in pressure.

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

field of view in the stratosphere and above. The longitudinal separation of MLS measurements from a given day, which is determined by the Aura orbit, is 10°–20° over middle and low latitudes, and finer in polar regions.

3.22.4 Precision

The precision of the MLS v5.0*x* temperature measurement is summarized in Table 3.22.1. Precision is the random component of measurements which would average down if the measurement were repeated. The retrieval software returns an estimate of precision based upon the propagation of radiometric noise and *a priori* uncertainties through the measurement system. These values, which range from 0.5 K in the lower stratosphere to ∼2.5 K in the mesosphere and 4 K at 0.00046 hPa, are given, for selected levels, in column 2. Column 3 gives the root-mean-square of differences of values from successive orbits (divided by the square-root of two as we are looking at the difference of two noisy signals) for latitudes and seasons where longitudinal variability is small and/or is a function only of local solar time. The smallest values found, which are in the tropics in the troposphere and in high-latitude summer in the stratosphere and mesosphere, are taken to be those least impacted by atmospheric variability and are what is reported in column 3. These values are 0.5–0.8 K larger than those estimated by the measurement system in the troposphere and lower stratosphere, and a factor of ∼1.4 larger from the middle stratosphere through the mesosphere.

3.22.5 Accuracy

A substantial study was made of sources of systematic error in MLS v4.2*x* measurements, similar to that which was done as a part of the validation of v2.2. The accuracy of the v5.0*x* temperature measurements should be nearly identical to that of v4.2*x*. This accuracy was estimated both by modeling the impact of uncertainties in measurement and retrieval parameters that could lead to systematic errors, and through comparisons with correlative data sets. Column 5 of Table 3.22.1 gives estimates from the propagation of parameter uncertainties, as discussed in *Schwartz et al.* [2008]. This estimate is broken into two pieces. The first term was modeled as amplifier non-linearity, referred to as "gain compression," and was believed to have a known sign, as gain is known to drop at high background signal levels. Correction of these nonlinearities was a goal of v4.2*x*, but closer examination of the simple non-linearity model found that it did not close forward model and measured radiances as expected. It had been hoped that better radiance closure would permit the use of more radiances in the middle of the 118-GHz O_2 band, giving better resolution, precision and accuracy in the upper stratosphere and better accuracy everywhere. This work is still ongoing, and it is hoped that advances will manifest in improvements in a future version.

The second term of column 5 combines 2σ estimates of other sources of systematic uncertainty, such as spectroscopic parameters, retrieval numerics and pointing, for which the sign of resulting bias is unknown. Gain compression terms range from −1.5 K to +4.5 K, and predicted vertical structure is similar to observed biases relative to correlative data in the troposphere and lower stratosphere. The terms of unknown sign are of ∼2 K magnitude over most of the retrieval range, increasing to 5 K at 261 hPa and to 3 K at 0.001 hPa.

Column 6 contains estimates of bias based upon comparisons with analyses and with other previously-validated satellite-based measurements. In the troposphere and lower stratosphere, the observed biases between MLS and most correlative data sets are consistent to within ∼1.5 K, and have vertical oscillation with an amplitude of 2–3 K and a vertical frequency of about 1.5 cycles per decade of pressure. A global average of correlative measurements is shown in Figure 3.22.5.

3.22.6 Data screening

Pressure range: 261–0.00046 hPa

Values outside this range are not recommended for scientific use.

Estimated precision: Only use values for which the estimated precision is a positive number.

Values where the *a priori* information has a strong influence are flagged with negative or zero precision, and should not be used in scientific analyses (see Section 1.5).

Status flag: Only use profiles for which the `Status` field is an even number.

Odd values of `Status` indicate that the profile should not be used in scientific studies. See Section 1.6 for more information on the interpretation of the `Status` field.

Quality: Only use profiles with `Quality` greater than 0.2 for the 83 hPa level and smaller pressures, and profiles with `Quality` greater than 0.9 at larger pressures of 100 hPa and larger.

Profiles with `Quality` less than or equal to 0.9 comprise 1.4% of all data, and 4.8% of profiles in the tropics.

Convergence: Only profiles whose `Convergence` field is less than 1.03 should be used.

This `Convergence` criterion rejects $< 0.1\%$ of profiles and chunks with convergence slightly over this target do not contain manifestly pathological profiles. The primary purpose of this criterion is to reject profiles with extremely poor convergence that may be expected to reflect poor retrieval behavior.

Cloud Screening: The "low cloud" bit of the temperature `Status` field does not contain useful information in v5.0*x*, so it cannot be used to screen temperature as it was in version v03.2. However, cloud impacts can largely be removed using the ice water content (IWC) product, rejecting profiles between 261–100 hPa for which the 215 hPa value of IWC is greater than 0.005 g/m^3. Implementation of this criteria requires the loading of the v5.0*x* IWC swath, but is responsible for most of the rejection of cloud-induced outliers seen in Figure 3.22.3. This criteria removes 4.7% of UT profiles globally and 15% of profiles in the tropics (20°N–20°S).

Precision: The `L2gpPrecision` field can be used to further eliminate outliers that are believed to be the result of thick clouds, primarily in the tropics. If careful screening of the troposphere is required, levels 261–178 hPa should be avoided if any of the following criteria are met:

At 316 hPa: `L2gpPrecision` > 1.1 K **and** latitude > -60

At 261 hPa: `L2gpPrecision` > 0.7 K

At 215 hPa: `L2gpPrecision` > 0.825 K

3.22.7 Artifacts

MLS temperature has persistent, vertically oscillating biases with respect to analysis and correlative measurements in the troposphere and stratosphere that are an area of continued research. The impact of clouds is generally limited to tropospheric levels and to the tropics and, to a lesser extent, mid-latitudes. Cloud impacts in unscreened data at the lowest retrieved levels are larger in v5.0*x* than they were in v4.2*x* and are harder to screen due to the lack of a useful "low cloud" status bit. However, after recommended screening, tropical negative departures from *a priori* of greater than 10 K (believed almost always to cloud-induced artifacts) are seen in only 0.2% of tropical profiles. Flagging of clouds is discussed above. Further discussion of artifacts may be found in *Schwartz et al.* [2008].

3.22.8 Review of comparisons with other datasets

Schwartz et al. [2008] describe detailed comparisons of MLS v2.2 temperature with products from the Goddard Earth Observing System, version 5 [*Rienecker et al.*, 2007] (GEOS-5), the European Center for Medium-Range Weather Forecast [e.g., *Simmons et al.*, 2005] (ECMWF), the CHAllenging Minisatellite Payload (CHAMP) [*Wickert et al.*, 2001], the combined Atmospheric Infrared Sounder / Advanced

Help Overview Table BrO CH_3Cl CH_3CN CH_3OH ClO CO GPH H_2O HCl HCN HNO_3 HO_2 HOCl IWC IWP N_2O O_3 OH RHI SO_2 T Lvl 3

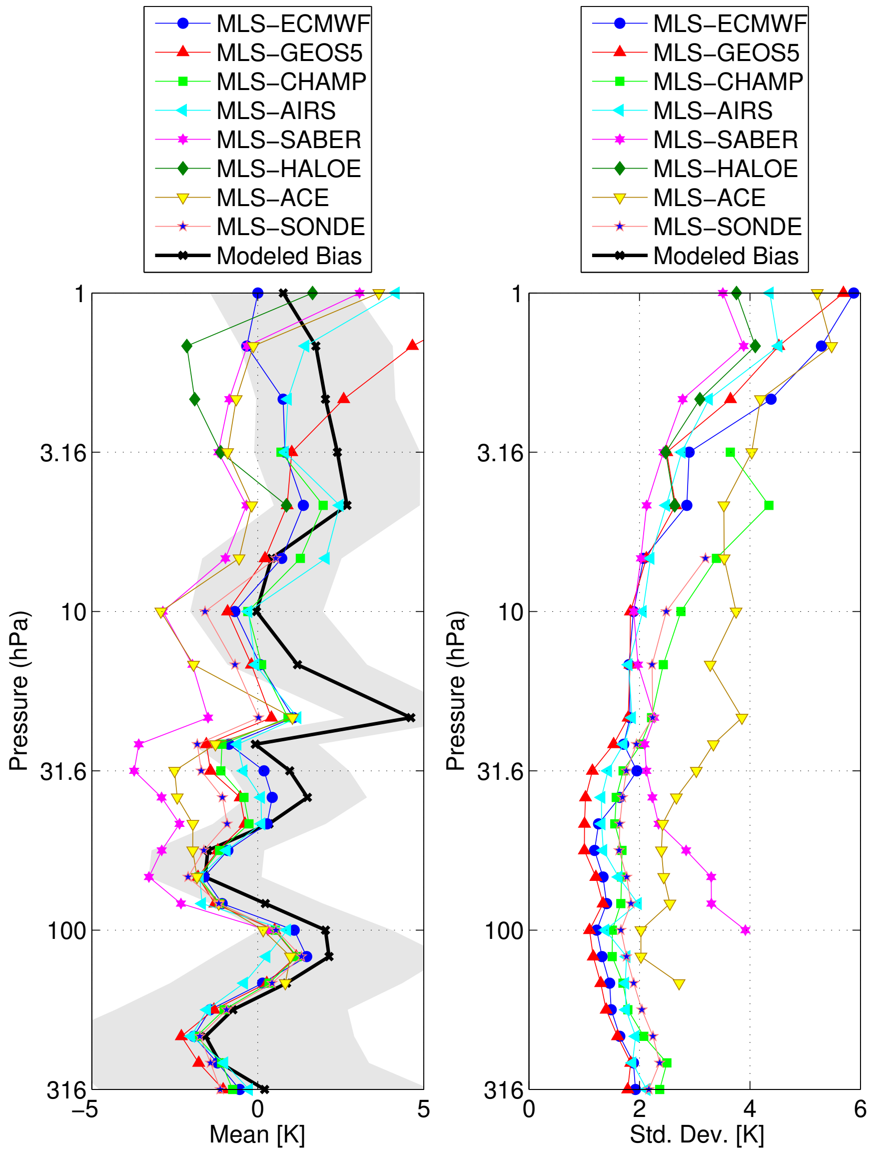

Figure 3.22.5: The left panel shows globally-averaged mean differences between MLS v4.2x temperature and eight correlative data sets. Criteria for coincidences are described in detain in Schwartz et al. [2008]. The right panel shows the global standard deviations about the means.

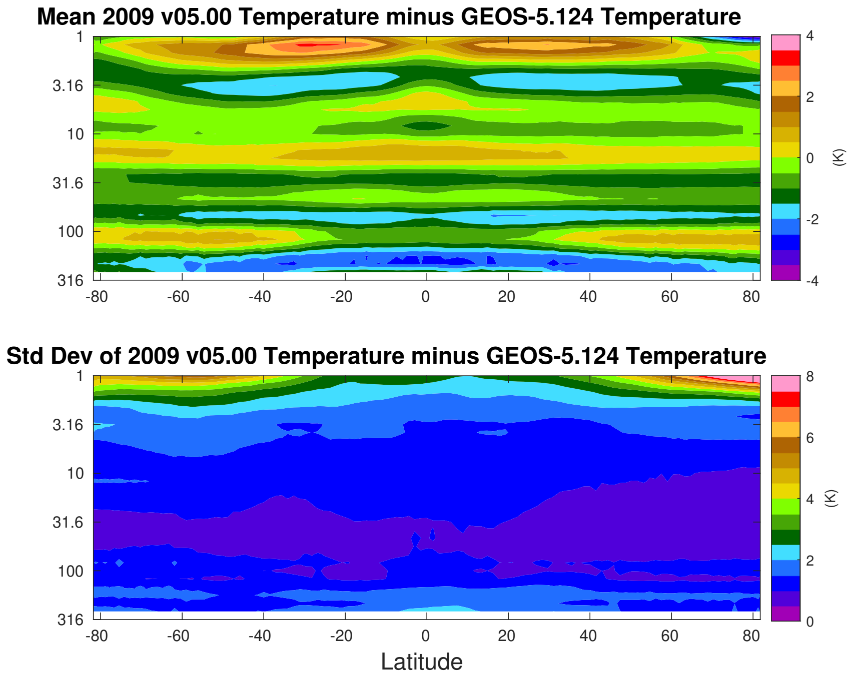

Figure 3.22.6: Zonal mean of the difference between MLS v5.0x temperature and GEOS-5 temperature (upper), and variability about that mean (lower), averaged for 2009. Y-axes are pressure in hPa.

Microwave Sounding Unit (AIRS/AMSU), the Sounding of the Atmosphere using Broadband Radiometry (SABER) [*Mlynczak and Russell*, 1995], the Halogen Occultation Experiment [*Hervig et al.*, 1996] (HALOE) and the Atmospheric Chemistry Experiment [*Bernath et al.*, 2004] (ACE), as well as to radiosondes from the global network. From 261 hPa to ~10 hPa there is generally agreement to ~1 K between the assimilations (ECMWF and GEOS-5) and AIRS, radiosondes and CHAMP, with SABER and ACE having generally warm biases of ~2 K relative to this group. Figure 3.22.5 shows the global mean biases in the left panel and the 1σ scatter about the mean in the right panel for these eight comparisons. Between 1 hPa and 0.001 hPa, MLS has biases with respect to SABER of +1 K to −5 K between 1 hPa and 0.1 hPa, of 0 K to −3 K between 0.1 K and 0.01 K and increasing in magnitude to −10 K at 0.001 hPa. Estimates of systematic error in the MLS temperature are shown in black, with 2σ uncertainty shown with gray shading. The black line is the modeled contribution of "gain compression," which was hoped would explain much of the vertical structure of MLS biases in the upper troposphere and lower stratosphere. As discussed above, the gain-compression model used in this study does not adequately close the retrieval's radiance residuals, so further study is needed to understand the forward-model inadequacies.

The upper panel of Figure 3.22.6 shows zonal-mean differences between v5.0*x* temperature and GEOS-5 temperature, averaged over 2009; the lower panel is the 1σ variability about that mean. Persistent vertical structure in the troposphere and lower stratosphere is evident, with the oscillations somewhat stronger at the equator and poles than at mid-latitudes. In the upper stratosphere, MLS has a general warm bias relative to GEOS-5 at mid and high latitude that increases to more than 10 K in the poles at 1 hPa. The bias at 1 hPa is much smaller in polar summer, but persists in polar winter.

Table 3.22.1: Summary of MLS Temperature product

Pressure	Precision[a] / K	Observed Scatter[b] / K	Resolution V × H / km	Modeled accuracy / K	Observed accuracy / K	Comments
<0.00022 hPa	—	—	—	—	—	Unsuitable for scientific use
0.00022 hPa	±5.1	—	12 × 370	—	—	Further validation needed. Generally not useful.
0.00046 hPa	±4.0	—	13 × 316	—	—	Further validation needed. Use with caution.
0.001 hPa	±3.6	±3.5	12 × 280	+2 ± 1	−9	
0.01 hPa	±3.4	±3	11 × 250	+2 ± 1	−2 to 0	
0.1 hPa	±2.5	±2.7	6.4 × 170	+3 ± 1.2	−8 to 0	
0.316 hPa	±1.3	±1.5	8.1 × 170	+2 ± 0.8	−7 to −4	
1 hPa	±1.2	±1.3	6.8 × 165	+1 ± 0.5	0 to +5	
3.16 hPa	±0.8	±0.8	5.5 × 165	+2 ± 1.2	+1	
10 hPa	±0.6	±0.7	4.1 × 165	−1 ± 0.5	−1 to 0	
14.7 hPa	±0.6	±0.7	3.9 × 165	+2.7 ± 0.9	0 to +1	
31.6 hPa	±0.5	±0.6	3.6 × 165	+0.7 ± 0.7	−2 to 0	
56.2 hPa	±0.6	±0.7	3.7 × 165	−1.5 ± 0.8	−2 to 0	
100 hPa	±0.7	±1.0	4.6 × 165	+1.8 ± 1.2	0 to +1	
215 hPa	±0.8	±1.2	3.5 × 165	−0.8 ± 1.4	−2.5 to −1.5	
261 hPa	±0.6	±1.5	3.8 × 167	0.4 ± 2.4	−2 to 0	
1000–316 hPa	—	—	—	—	—	Unsuitable for scientific use

[a]Precision on individual profiles

[b]Precision inferred from differences of individual profiles from successive orbits (v2.2 results shown)

Chapter 4
MLS Level 3 datasets

4.1 Introduction

The other chapters of this guide describe MLS “Level 2” data – geophysical products along the instrument observing track. This chapter describes MLS “Level 3” data – geophysical products binned onto regular grids. There is a wide array of techniques for transforming along-track observations into regular grids, including “kriging” approaches [e.g., *Cressie*, 2015], Fourier-series-based approaches [*Salby*, 1982], approaches using various windowing functions such as Hamming windows, and simple binning approaches. All methods have strengths and weaknesses, and the choice of which one to use is best made by the individual data user, based on the nature of the specific scientific question to be tackled. For this reason, until 2020, the MLS team had not produced any “official” Level 3 data products.

However, in order to facilitate certain studies by MLS data users, the MLS team is now producing and distributing a select set of Level 3 products derived using a simple “binning” approach (i.e., simply reporting the mean measured value within a given spatial/temporal “box”). As part of the generation of these data products, all the data screening rules described in chapters 1 and 3 are applied (along with the ClO bias correction, see section 3.6), providing a significant additional simplification to data users. Level 3 data are supplied for most MLS standard products. BrO and HO_2 are excluded, as they have have a different Level 3 product available (see sections 3.2 and 3.13). We also exclude CH_3CN and CH_3OH in light of the narrow range over which these products are recommended for scientific use.

Three sets of Level 3 products are provided:

Daily Binned Files: These are stored as one product per day of MLS data per file. The daily binned files contain the following datasets:

- Geodetic latitude and longitude maps on a pressure vertical coordinate (i.e., “3D” fields).
- Geodetic latitude and longitude maps on a potential-temperature vertical coordinate (i.e., “3D” fields).
- Geodetic latitude zonal means on a pressure vertical coordinate (“2D”).
- Geodetic latitude zonal means on a potential-temperature vertical coordinate (“2D”).
- Equivalent latitude[1] “zonal means” on a potential-temperature vertical coordinate (“2D”).
- Vortex averages on a potential-temperature vertical coordinate (“1D”).

Monthly Binned Files: These are stored as one product per year of MLS data per file. The monthly binned files contain the same datasets as the daily binned files, except with twelve monthly entries in each dataset instead of one daily one.

Zonal Mean Binned Files: These files contain “roll-ups” of all the datasets in the daily binned files, excluding the “3D” maps. These are provided with fields having 365 or 366 entries per dataset in each file.

For species with non-negligible diurnal variations over all or part of their vertical range (ClO, OH, HOCl, and O_3), the datasets described above are further subdivided into five different datasets containing:

[1] Equivalent latitude is the geographical latitude that encloses the same area as an isoline of potential vorticity, giving a polar vortex-centered latitude [*Butchart and Remsberg*, 1986].

- All valid profiles (as for all the non-diurnal products).
- All profiles measured on the ascending side of the orbit (mainly daytime observations, except in polar regions).
- All profiles measured on the descending side of the orbit (mainly nighttime observations, except in polar regions).
- All observations made with solar zenith angle less than 90° (i.e., daytime observations).
- All observations made with solar zenith angle greater than 110° (i.e., nighttime observations).

MERRA-2 [*Gelaro et al.*, 2017] reanalysis temperature fields (interpolated to each MLS observation point) are used to convert from pressure to potential temperature surfaces. Additionally MERRA-2 potential vorticity fields are used to construct equivalent latitude and vortex average information. The interpolated MERRA-2 fields used are taken from the MLS "Derived Meteorological Products" [*Manney et al.*, 2007, 2011]. Note that, for quantities on potential temperature surfaces, the MLS Level 3 profiles on pressure levels are first interpolated to the fixed potential temperature surfaces (from $\log[p]$ to $\log[\theta]$) before being binned (as opposed to directly binning Level 3 data points in potential temperature windows, which has the potential to introduce undesirable empty bins in the vertical). These interpolated values (and the interpolated `L2GPPrecision` field) are then used to construct all fields.

The vortex averages are defined using an altitude-dependent value of scaled potential vorticity (sPV) to demark the vortex edge. The values at each level are determined separately for each hemisphere, using the prodedure described by *Lawrence et al.* [2018] wherein a constant sPV for each hemisphere and season is derived based on the climatological sPV at the location of the maximum high-latitude sPV gradient. While there are numerous methods of estimating the location of the vortex edge, this simple method with a value that is constant in time has been shown to avoid some common pitfalls such as large spurious day-to-day changes in vortex area and inappropriate values at the beginning and end of the cold season [see *Lawrence and Manney*, 2018, for a discussion of pros and cons of various vortex edge identification methods]. To estimate uncertainties in vortex edge definition, and to provide results for studies where more or less conservative estimates of the vortex edge are desirable, averages are also provided for "outer" and "inner" vortex edge values that are $0.2\times10^{-4}\text{s}^{-1}$ less and more, respectively, than the determined value for the vortex edge "center" [this also follows *Lawrence et al.*, 2018].

4.2 Level 3 data files

Two different temporal resolutions of Level 3 data are provided—daily (`L3DB`) and monthly (`L3MB`). The `L3DB` files are one file per day per Level 3 data product (with one time entry in each dataset in the file), and the `L3MB` files are one file per year per Level 3 data product (with twelve time entries in each dataset in the file). Both of these files contain latitude/longitude grids, zonal means, and polar vortex averages on various vertical coordinates, as described in section 4.1, above. To aid in the analysis of long-term datasets, the additional `L3DZ` files are a yearly rollup of all of the `L3DB` datasets except for the latitude/longitude grids, which are not included for file size considerations. The datasets in `L3DZ` files contain 365 or 366 time entries as appropriate. The filenames for these products using the following conventions, which differ mainly in the date format:

`MLS-Aura_L3DB-<product>_v04-20-c01_<yyyy>d<ddd>.nc`
`MLS-Aura_L3MB-<product>_v04-20-c01_<yyyy>.nc`
`MLS-Aura_L3DZ-<product>_v04-20-c01_<yyyy>.nc`
`MLS-Aura_L3MB-<product>_v04-20-c01_<yyyy>m<mm>.nc` (Mid-year forward processing only)
`MLS-Aura_L3DZ-<product>_v04-20-c01_<yyyy>m<mm>.nc` (Mid-year forward processing only)

Where
<product> is the MLS standard product: CO, O3, Temperature, etc.
<yyyy> is the four-digit year
<ddd> is a three-digit day of year <ddd> (001 = 1 January)
<mm> is an optional two-digit month for monthly files.

Files using the two-digit month will only be available during their current calendar year, as "forward processing" data are gathered, and will contain all data in the year up to and including the quoted month, with the remaining date entries present but consisting of values marked "bad" (i.e., with the netCDF _FillValue). Once all months are available, the complete dataset will be stored in the "<yyyy>" files.

Within each file, the datasets are stored in netCDF-4 groups. The L3DB and L3MB files contain six types of datasets: latitude/longitude grids on both pressure and potential temperature vertical coordinates, zonal means on both pressure and potential temperature vertical coordinates, means within equivalent latitude contours on potential temperature surfaces, and polar vortex averages as a function of potential temperature. As noted above, the L3DZ files omit the latitude/longitude maps.

These datasets are named as follows (where <product> is the same as listed in the filename):

<product> PressureGrid:	4°×5° geodetic longitude/latitude grid on pressure surfaces (L3DB and L3MB only)
<product> ThetaGrid:	4°×5° geodetic longitude/latitude grid on potential temperature surfaces (L3DB and L3MB only)
<product> PressureZM:	4° geodetic latitude zonal mean on pressure surfaces
<product> ThetaZM:	4° geodetic latitude zonal mean on potential temperature surfaces
<product> EqLZM:	4° equivalent latitude zonal mean on potential temperature surfaces
<product> VortexAvg:	Polar vortex average values for each hemisphere on potential temperature surfaces. The values are calculated in accordance with the "outer", "center", and "inner" vortex edge criteria documented in *Lawrence et al.* [2018].

Diurnal product files have all of these groups repeated for day, night, ascending profiles only, and descending profiles only (with Day, Night, Asc, Desc, respectively added to the group name).

Each group contains the following data fields:

lon:	The longitude at center of the grid cell (PressureGrid and ThetaGrid groups only)
lon_bnds:	The longitude at the boundaries of the grid cell (PressureGrid and ThetaGrid groups only)
lat:	The latitude at center of the grid cell
lat_bnds:	The latitude at the boundaries of the grid cell
time:	The date of the grid cell (days since 1950-01-01)
time_bnds:	The boundaries of the time period (days since 1950-01-01)
lev:	The vertical coordinate (i.e. pressure/potential temperature values)
value:	The average value for each bin
nvalues:	The number of valid data points found in each bin
rms_uncertainty:	The root mean square of all the Level 2 L2GPPrecision values that contributed to each bin (note that this has *not* been divided by $\sqrt{\texttt{nvalues}}$)
minimum:	The minimum value in each bin
maximum:	The maximum value in each bin
std_dev:	The standard deviation of the data in each bin

4.3 Guidance for users of Level 3 data

As discussed above, these Level 3 products are generated using only the Level 2 data points that meet all the screening criteria described in the earlier chapters of this document, providing a significant simplification for users. In cases where there are no good Level 2 data available to populate a Level 3 data point, the `nvalues` field is set to zero and the other data fields are set to the `_FillValue` (bad data flag) for the given netCDF variables.

When considering Level 3 data, as with every geophysical measurement, attention should be paid to the associated uncertainties. The averaging inherent in generating Level 3 data will act to reduce "precision"-related errors, those due to random noise in the MLS radiance measurements, by $1/\sqrt{n}$, where n is the number of Level 2 data points in the average (which is given by the `nvalues` field). We have chosen not to divide by $\sqrt{n}$ in the files in order to make it easier for users who wish to perform further averaging. For example, when creating weekly averages from the daily L3 data, the final precision can be computed as the root-mean-square of the daily precisions divided by the square root of the total of the daily `nvalues` entries.

In contrast, the "accuracy"-related errors, those due to biases in the MLS measurement system, will in most cases be propagated through the averaging process unchanged, and should be assumed to apply to the Level 3 values in the same manner as they do to the values in the underlying Level 2 datasets.

Appendix A
Embedded data files

In part to comply with journal requirements for data availability, and also to help assure long-term preservation of key datasets beyond the lifetime of the MLS project, selected data files are embedded in the PDF version of this document, and can be extracted as described below.

Not all PDF readers support the file-extraction capability. At the time of writing, the "Adobe Reader" software provides the needed functionality. File extraction can be accomplished through a "right click" (or some similar action, such as "option-click") on the icons below, and selecting the "Save Embedded File to Disk..." option.

A.1 Averaging kernels

The MLS averaging kernels are also available for download from the MLS website at `https://mls.jpl.nasa.gov/eos-aura-mls/data-products/averaging-kernels` as a single tar-archive.

	70°S	35°S	Equator	35°N	70°N
1D kernels					
2D kernels					

A.2 ClO bias correction

Per the discussion in section 3.6, biases in lower-stratospheric ClO can be corrected to first order by subtracting the values given in this file , which is also available at `https://mls.jpl.nasa.gov/data/MLS-Aura_ClO-BiasCorrection_v05.txt`

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