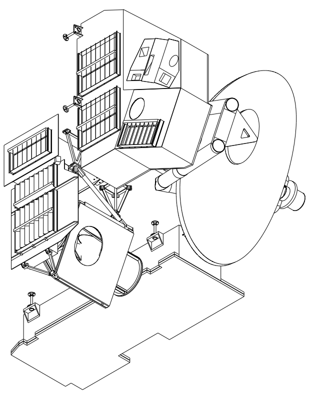
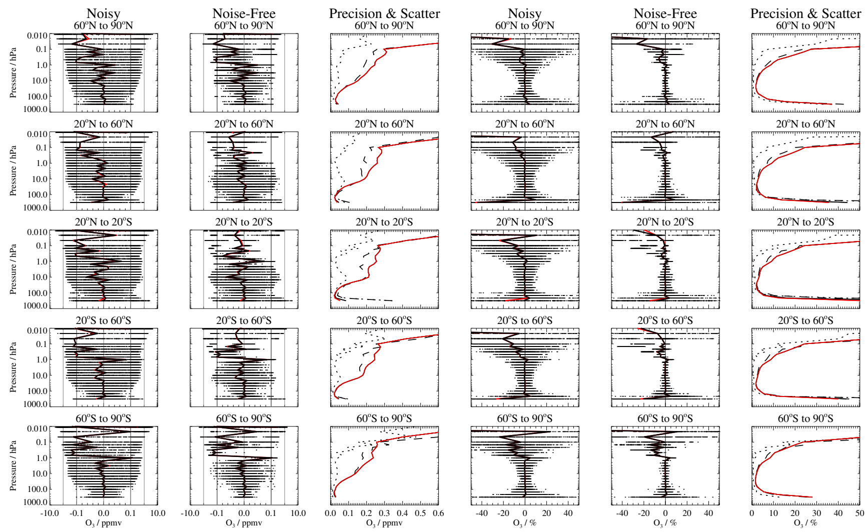
JPL D-32381

Earth Observing System (EOS)

Microwave Limb Sounder (MLS)

Version 1.5 Level 2 data quality and description document.





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Where to find answers to key questions

This document serves two purposes. Firstly, to summarize the quality of version 1.5 (v1.5) EOS MLS Level 2 data. Secondly, to convey important information on how to read and interpret the data to the scientific community.

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, after a few pages of introduction, 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 v1.5 MLS Level 2 data?

All the MLS Level 2 data described here can be obtained from the NASA Goddard Space Flight Center Distributed Active Archive Center (GSFC-DAAC, see `http://daac.gsfc.nasa.gov/`). EOS MLS data are also available from the *Aura Validation Data Center* (AVDC, `http://avdc.gsfc.nasa.gov/`), along with a growing number of validation datasets (or pointers thereto).

What format are MLS Level 2 data files in. How do I read them?

MLS Level 2 data are in HDF-EOS version 5 format. Details are given in section 1.3 (page 3).

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

These issues are described in section 1.4 (starting on page 4), 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 this precision is set negative to indicate 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 non zero should be approached with caution. See section 1.4 on page 4, 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 lower than the threshold given in the section of chapter 3 describing your product of interest.
- Detailed discussion of the accuracy of these data is not included in this document as the formal 'validation' process is incomplete at the time of writing. More details will be given in forthcoming MLS validation papers.
- As always, 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.

Contents

Acknowledgment

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Chapter 1
Essential reading for users of MLS version 1.5 data

1.1 Scope and background for this document

This document describes the quality of the geophysical data products produced by version 1.5 (v1.5 hereafter) of the data processing algorithms for the EOS Microwave Limb Sounder (MLS) instrument on the Aura spacecraft. The intended audience is those wishing to make use of EOS MLS data for scientific study. The geophysical products described in this document are all produced by the "Level 2" algorithms, and briefly summarized in Table 1.1. The v1.5 dataset is the first set of data considered suitable for general scientific use. The detailed validation of these products is still underway and will be described in later publications. As always, those wishing to use MLS data are strongly advised to consult the MLS science team concerning their intended use.

In addition to describing the data quality, this document gives a brief outline of the algorithms used to generate these "Level 2" data (geophysical products reported along the instrument track) from the input "Level 1" data (calibrated microwave radiance observations).

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] is a very useful source of information on the expected precision of the EOS MLS data, and should be regarded as a companion volume to this document. 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 these documents are available from the MLS web site (`http://mls.jpl.nasa.gov/`). A series of papers has been submitted to the IEEE Transactions on Geoscience and Remote Sensing. An overview of MLS is given in Waters et al. [2005], the algorithms that produce the data described here are reviewed in Livesey et al. [2005]; Read et al. [2005]; Schwartz et al. [2005]; Wu et al. [2005]. Some early v1.5 validation studies are described in Froidevaux et al. [2005]. Other papers in that issue describe the calibration and performance of the various aspects of the MLS instrument [Jarnot et al., 2005; Pickett, 2005; Cofield and Stek, 2005] and the MLS ground data system [Cuddy et al., 2005].

1.2 Overview of v1.5 and this document

The remainder of this chapter reviews issues that are considered *essential reading* for users of the v1.5 dataset. Chapter 2 details relevant aspects of the MLS instrument design and operations and the theoretical basis for the v1.5 algorithms that are considered *background reading*.

Chapter 3 describes the data quality to be expected for "Standard" products from the MLS instrument for v1.5. These are observations of vertical profiles of the abundance of BrO, ClO, CO, H_2O, HCl, HCN, HNO_3, HO_2, HOCl, N_2O, O_3, and OH, along with temperature, geopotential height, relative humidity (deduced from the H_2O and temperature data), and cloud ice water content, all described as functions of pressure. In v1.5 these profiles are output on a grid that has a vertical spacing of six surfaces per decade change in pressure ($\sim$2.5 km),

Table 1.1: Key information for each MLS standard product. All standard product files for species abundances also contain estimated column loading above the tropopause (WMO definition) determined from the MLS temperature data. See the text for details on the meaning of the various columns.

Product name	Useful range	*Significant* averaging needed?[a]	Quality threshold[b]	Differences needed?[c]	Cloud impact [d]	Contact name	Contact Email
BrO	10 – 2.2 hPa	yes	1.0	yes	none	Nathaniel Livesey	livesey@mls.jpl.nasa.gov
CH3CN[e]	Unclear	N/A	N/A	N/A	N/A	Nathaniel Livesey	livesey@mls.jpl.nasa.gov
ClO	100 – 1.0 hPa	no	2.7	see text	none	Michelle Santee	mls@mls.jpl.nasa.gov
CO	215 – 0.0046 hPa	no	0.05	no	$p \geq 100$ hPa	Mark Filipiak	M.J.Filipiak@ed.ac.uk
GPH[f]	316 – 0.001 hPa	no	see text	no	none	Michael Schwartz	michael@mls.jpl.nasa.gov
H2O	316 – 0.1 hPa	no	0.02[g]	no	$p \geq 100$ hPa	William Read (trop.) Hugh Pumphrey (strat./mes.)	bill@mls.jpl.nasa.gov H.C.Pumphrey@ed.ac.uk
HCl	100 – 0.22 hPa	no	1.5	no	none	Lucien Froidevaux	lucien@mls.jpl.nasa.gov
HCN	10 – 1.4 hPa	no	1.0	no	none	Hugh Pumphrey	H.C.Pumphrey@ed.ac.uk
HNO3	147 – 3.2 hPa	no	0.17	no	none	Michelle Santee	mls@mls.jpl.nasa.gov
HO2	22 – 0.22 hPa	yes	2.5	yes	none	Herbert Pickett	hmp@mls.jpl.nasa.gov
HOCl	22 – 2.2 hPa	yes	1.3	no	none	Lucien Froidevaux	lucien@mls.jpl.nasa.gov
IWC[h]	215 – 68 hPa	no	N/A	no	N/A	Dong Wu Jonathan Jiang	dwu@mls.jpl.nasa.gov jonathan@mls.jpl.nasa.gov
N2O	100 – 0.1 hPa	no	2.5	no	none	Nathaniel Livesey	livesey@mls.jpl.nasa.gov
O3	215 – 0.46 hPa	no	0.1	no	$p \geq 100$ hPa	Mark Filipiak (trop.) Lucien Froidevaux (strat./mes.)	M.J.Filipiak@ed.ac.uk lucien@mls.jpl.nasa.gov
OH	46 – 0.2 hPa	no	0.5	no	none	Herbert Pickett	hmp@mls.jpl.nasa.gov
RHI[i]	316 – 0.1 hPa	no	see text	no	$p \geq 100$ hPa	William Read	bill@mls.jpl.nasa.gov
Temperature[j]	316 – 0.001 hPa	no	1.0	no	none	Michael Schwartz	michael@mls.jpl.nasa.gov

[a]Products marked 'yes' require significant averaging such as monthly zonal means to obtain useful signal to noise. Other products may require averaging for some of their vertical range, and/or particular latitudes/seasons to obtain the precision needed for individual studies.

[b]Discard profiles with `Quality` lower than this value.

[c]Day/night or ascending/descending differences required for suitable accuracy; see text for details.

[d]Thick clouds can have an impact on some MLS products in the troposphere. Typically 5 – 10% of profiles are affected, mainly in the tropics where 10 – 15% of the profiles are identified as having been affected by clouds.

[e]Not considered a 'standard product', not ready for scientific use.

[f]*Geopotential Height*

[g]Exceptions: use 0.3 for the 147 and 215-hPa data; use 5.0 for the 316-hPa data.

[h]*Ice Water Content*. This product has a reporting grid spaced at 12 surfaces per decade change in pressure.

[i]*Relative Humidity with respect to Ice*. Computed from the MLS H_2O and Temperature data.

[j]File also contains estimate of tropopause pressure (WMO definition) inferred from MLS temperatures.

thinning out to three surfaces per decade above 0.1 hPa (cloud ice is an exception to this, having a finer vertical grid). Horizontally the profiles are spaced by 1.5° great-circle angle along the orbit, which corresponds to about 160 km. The true vertical and 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 discussed in Appendix A which can be found in a supplement to this report.

At the time of writing, the current version of the data processing software is version 1.51, producing files labeled `v01-51`. The differences between the earlier version 1.50 (not available from the GSFC DAAC) and 1.51 were minor 'bug fixes'. This document is intended to be applicable to any v1.5*x* MLS data. Revisions that represent more than a minor 'bug fix' will not be known as v1.5*x* and will be accompanied by a revised version of this document.

1.3 EOS MLS file formats, contents, and first order quality information

The standard and diagnostic products are stored in the EOS MLS *Level 2 Geophysical Product* (L2GP) 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 the *Open Channel Software Foundation* (`http://www.openchannelsoftware.org/`).

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

```
MLS-Aura_L2GP-<product>_v1-51_<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). The files contain an HDF-EOS swath given the same name as the product. In addition, the standard product files also contain swaths describing column abundances or tropopause pressures, as described in section 1.7 (note the caveats associated with the column products described in that section). As the files contain two 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. While this generally results in the desired result for most products ("`O3`" comes before "`O3 column`" for example), for temperature, the tropopause pressure swath "`TPPressureWMO`" will be read instead of the "`Temperature`" swath.

Each swath contains data fields `L2gpValue` and `L2gpPrecision`, which describe the value and precision of the data, respectively. Data points for which `L2gpPrecision` is set negative *should not be used*, as this flag indicates that the instrument and/or the algorithms have failed to provide 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 elapsed (including 5 subsequent leap seconds) since midnight universal time on 1 January 1993.

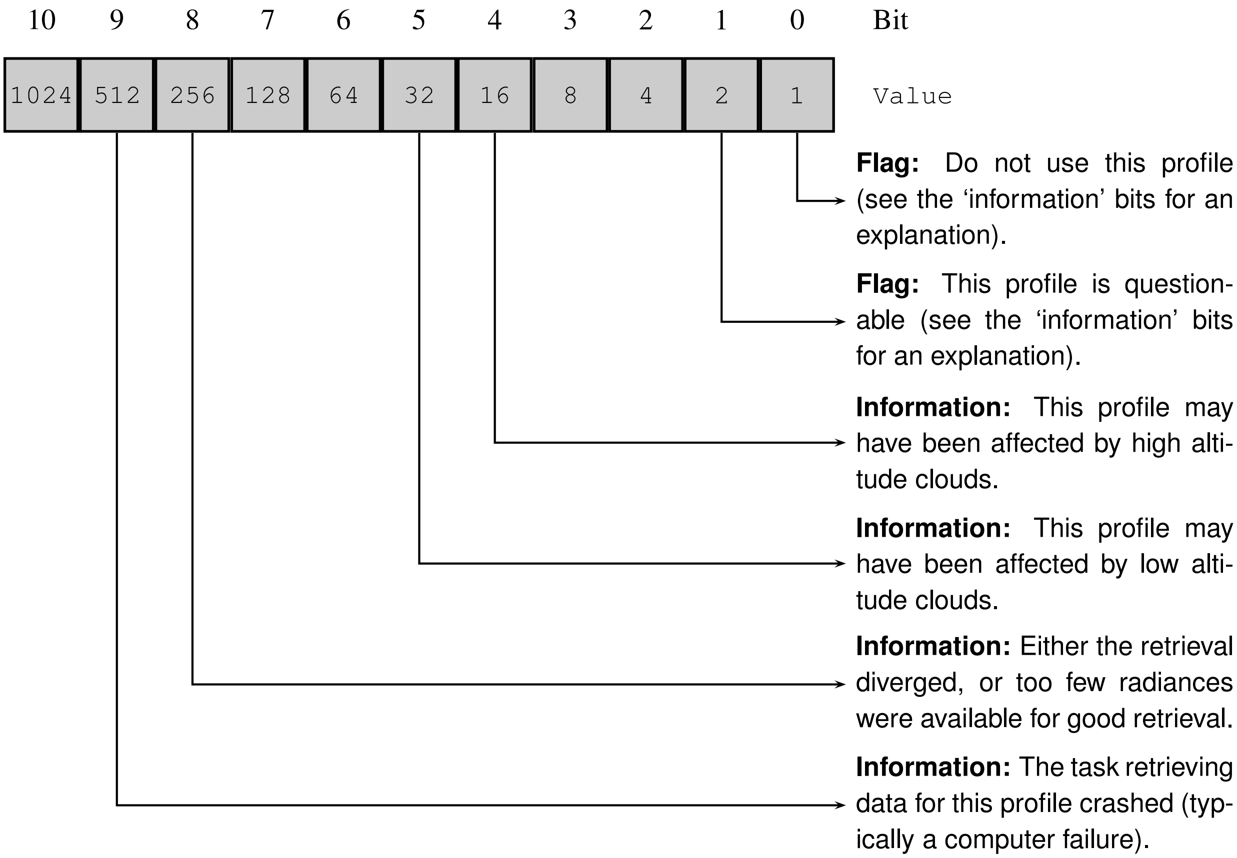


Figure 1.1: The meaning of the various bits in the `Status` field. The bits not labeled are not used in v1.5. Later versions may implement specific meanings for these bits.

1.4 Additional quality control information (`Quality` and `Status`)

In addition to the data and their estimated precisions, two 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 good radiance fits and therefore 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 "threshold" for rejecting data in scientific studies varies from product to product, and is given later in this document.

The other quality metric is called `Status`. This is a 32 bit integer that acts as a bit field containing several "flags". Figure 1.1 describes the interpretation of these flags in more detail. The first two bits (bits 0 and 1) are "flagging" bits. The first bit 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 indicates that data are considered questionable for some reason. Higher bits give more information on the reasons behind the setting of the first two bits. So, for example, a value of `Status` of `18` indicates that the data are questionable (`2`) because of the possible presence of high altitude clouds (`16`).

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 believed 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). The implications of this vary from product to product and, more importantly, height to height. For example, situations of "low cloud" 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.

1.5 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 1.6). Accordingly, no negative water vapor abundances are produced by v1.5. Studies involving averages in regions where the MLS signal to noise is poor (e.g., the mesosphere) should accordingly consider averages in log space.

1.6 The representation of MLS vertical profile observations

The MLS Level 2 data describe a piecewise linear representation of vertical profiles of mixing ratio (or temperature, or log mixing ratio for water vapor) 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 many other instruments, which report profiles in the form of discrete layer means. This interpretation has important implications that need to be considered when comparing profiles from MLS and other instruments, particularly those with higher vertical resolution.

It is clearly not ideal to compare MLS retrieved profiles with other data by simply 'sampling' the other profile at the MLS retrieval surfaces. One might expect that instead one should do some 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 turns out 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 $\mathbf{z}_h$. Let's describe that operation by the $n_h \times n_l$ matrix $\mathbf{H}$ such that

$$\mathbf{x}_h = \mathbf{H}\mathbf{x}_l \tag{1.1}$$

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

$$\mathbf{z}_l = \mathbf{W}\mathbf{z}_h \tag{1.2}$$

where

$$\mathbf{W} = \left[\mathbf{H}^{\mathrm{T}}\mathbf{H}\right]^{-1}\mathbf{H}^{\mathrm{T}} \tag{1.3}$$

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 1.2. Precision uncertainty on high resolution measurements may be similarly converted to the MLS grid by applying

$$\mathbf{S}_l = \mathbf{W}\mathbf{S}_h\mathbf{W}^{\mathrm{T}} \tag{1.4}$$

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.

In addition to this least squares operation, it is possible to multiply the high resolution data – as smoothed by the least squares operator – by the MLS averaging kernels. The two dimensional nature (vertical and along-track) of the MLS averaging kernels make this a complex task. Users wishing to embark on this exercise are

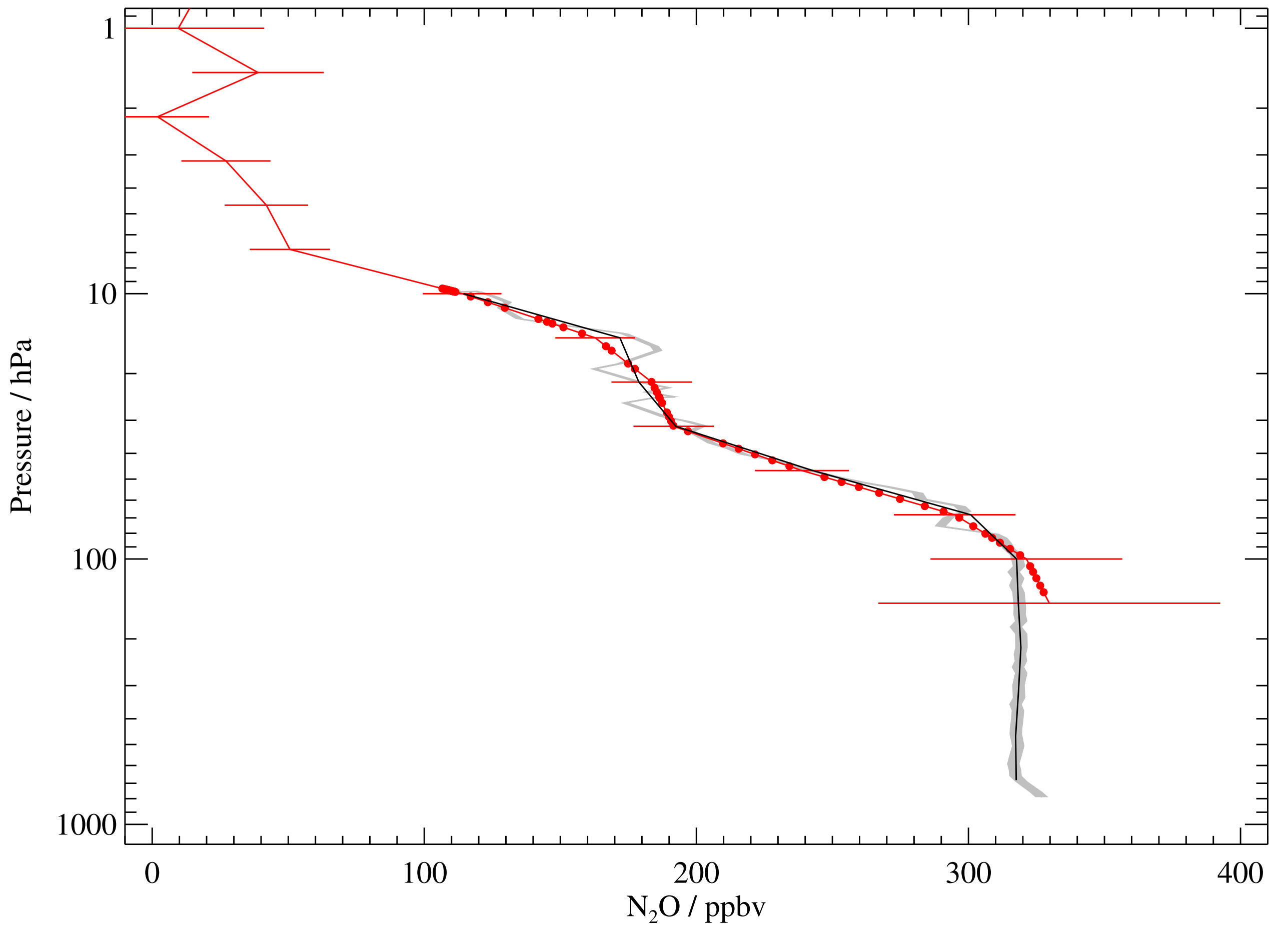


Figure 1.2: Comparisons of MLS v1.5 N_2O observations with in-situ balloon data (courtesy of J. Elkins). The raw balloon data ($\mathbf{z}_h$) are shown as the grey shaded region (shading indicates precision). A coincident MLS profile ($\mathbf{x}_l$) is shown in red with the red error bars indicating 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 1.1). 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 1.2). 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.

advised to contact the MLS science team for more information. As the averaging kernels for most MLS products are fairly sharply peaked, applying them usually makes only small differences to comparisons once the 'least squares' smoothing has been applied.

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.

1.7 Other quantities output by the software

The standard product files also include a swath containing an integrated column abundance of the product above the tropopause. These swaths have names such as `O3 column`. The pressure of the tropopause taken for the lower limit of the column is the WMO definition of the thermal tropopause (appropriately modified for pressure coordinates), obtained from the standard MLS temperature product. This pressure is output in the standard temperature file as a separate swath named `TPPressureWMO`. The WMO definition allows for the identification of two tropopauses within a profile, a common occurrence for Arctic winter profiles. The MLS software only reports the lowest altitude tropopause, which may not always be the appropriate choice. This leads to inappropriate behavior in the reported column abundances, as discussed further in section 3.15. Users are generally advised to form their own column abundance datasets from the MLS data using alternative data sources for the tropopause location.

Chapter 2
Background reading for users of MLS version 1.5 data

2.1 EOS MLS radiance observations

Figures 2.1 and 2.2 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 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 EOS MLS measurement system.

An innovative aspect of the retrieval algorithms for EOS MLS arises from taking advantage of the fact that the MLS instrument looks in the forward direction from the spacecraft. Figure 2.3 reviews the EOS MLS measurement geometry and shows that each radiance observation is influenced by the state of the atmosphere for several consecutive profiles. In the v1.5 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 1.6. 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

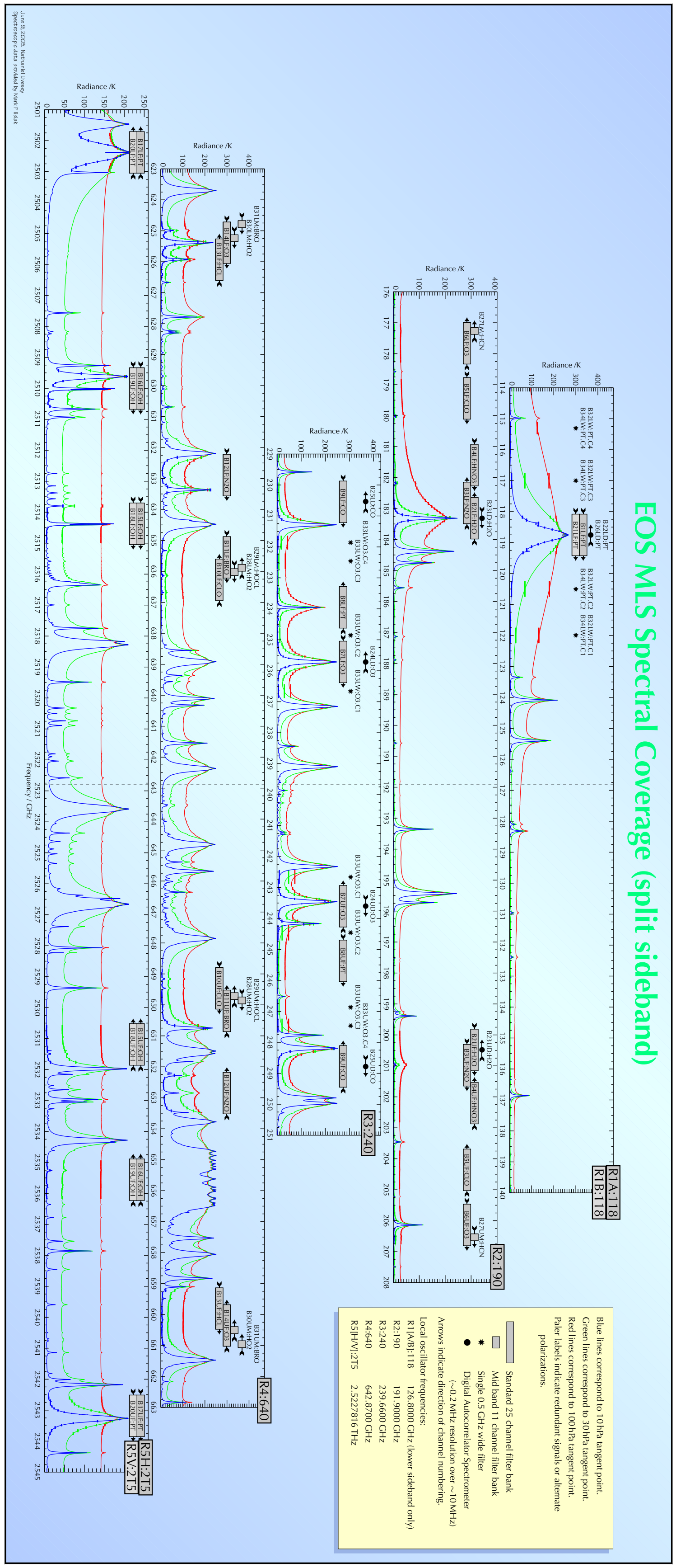


Figure 2.1: The five panels show the spectral regions covered by the MLS radiometers. The grey boxes and other symbols denote the position of the various "bands" observed within the spectral regions covered by each radiometer.

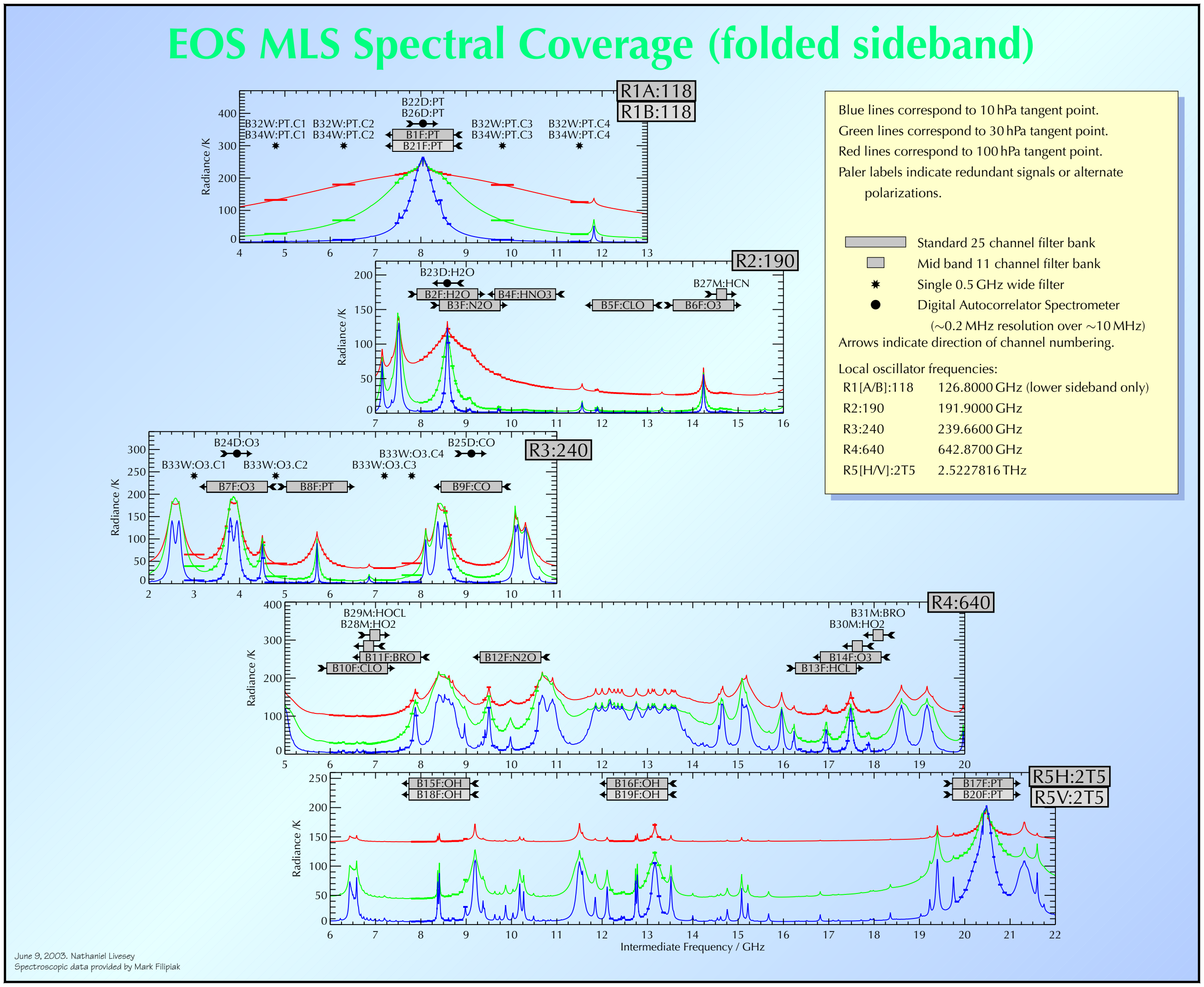


Figure 2.2: This is similar to figure 2.1, except that x-axes represent "intermediate frequency". The signal at each intermediate frequency represents a sum of the signals observed at that frequency both above and below the local oscillator.

measurement system manifest themselves as a spectrally flat error in radiance. This is true of both instrumental effects such as variations in instrument gain and offset during the limb scan, and "forward model" effects 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 v1.5 algorithms also retrieve spectrally flat corrections to the MLS radiances for each minor frame (typically one for each radiometer, though for R4, three are used, divided into broad spectral regions).

2.3 The Core, Core+Rn 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.

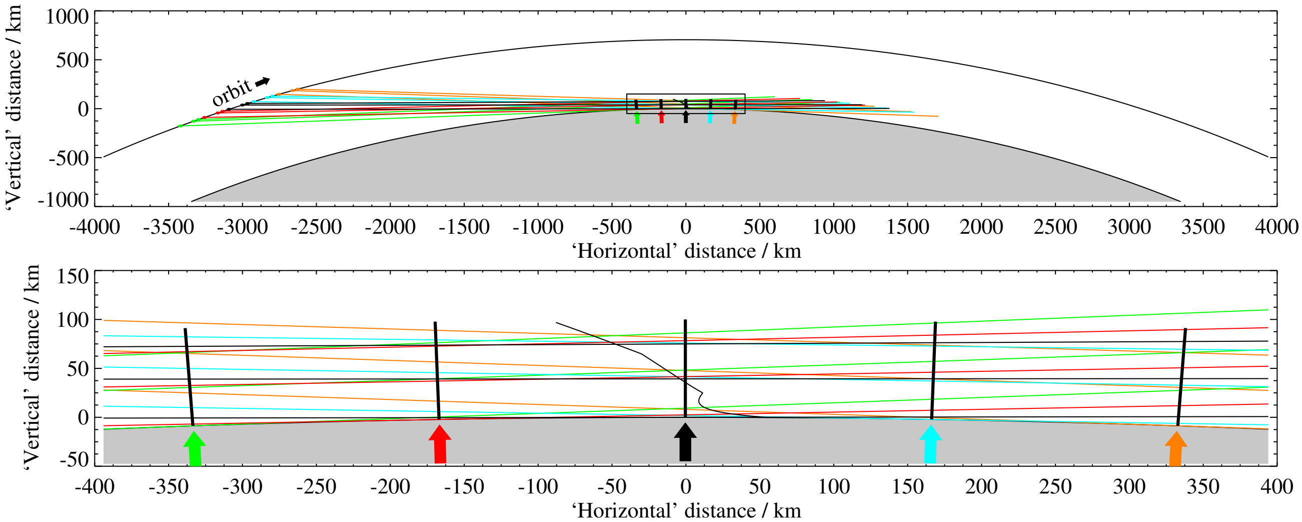


Figure 2.3: The top diagram shows a section of one orbit. Three of the 120 limb ray paths per scan are indicated by the "horizontal" lines. The lower diagram shows an expansion of the boxed region above. The straight radial lines denote the location of the retrieved atmospheric profiles. The limb ray 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.

However, there are some components of the state vector whose impact on the radiances is very 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 very non-linear. Solving for these aspects of the state vector will therefore require several iterations.

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*. For example, in the data processing for UARS MLS version 5 [Livesey et al., 2003], a retrieval phase of tangent pressure and temperature was followed by one of upper tropospheric humidity. Following those, retrieval phases were performed for other atmospheric species. These later phases used the values of tangent pressure, temperature and humidity established by the earlier phases in their forward model calculations. However, the knowledge of such parameters is uncertain (having come from an earlier retrieval), so if a correct error budget is to be maintained, the uncertainty in these parameters must be taken into account in the later retrievals. This accounting (known as *constrained quantity error propagation*) is typically a very time consuming process. In the case of EOS MLS, the effort involved is far too large to be realistically implemented in the algorithms, so an alternative approach is needed.

2.3.2 A new approach to retrieval phasing

For EOS MLS the retrievals still proceed in phases. However, in the later phases the previously retrieved quantities (e.g., tangent pressure, temperature etc.) are still retrieved, and the radiance measurements from which their earlier estimates were taken are still included in the measurement vector. Because the later phases now include the non-linear elements of the state vector, the retrieval error budget is correct. Furthermore, because the non-linear terms are presumably already close to their true values as a result of the earlier phase, in principal fewer iterations should be needed, as the system is closer to a linear regime.

This approach has been implemented in what is known as the "Core, Core+Rn" approach in the v1.5 algorithms. In the "Core" phase of the retrievals (actually three separate phases), retrieved estimates are obtained for the tangent pressure, temperature, and upper tropospheric humidity components of the state vector. These are obtained from the R1A 118 GHz observations of emission from O_2 (mainly for temperature and pressure) and selected channels from the R2 190 GHz observations (mainly for upper tropospheric water vapor). "Core" is followed by phases such as "Core+R2A", "Core+R2B", "Core+R3", ... where, in addition to temperature and pressure, other species such as ozone and nitric acid are retrieved. Version 1.5 includes a slight deviation from the plan outlined in the previous paragraph, in that water vapor (notably in the upper troposphere) is not retrieved in the phases after Core+R2A. It was found that including this term often led to instability in the later retrievals. Neglecting this term and its impact on the error budget (constrained quantity error propagation being out of the question) is not felt to have a significant impact on other v1.5 products.

Table 2.1 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 Core+R2B retrieval is known in the v1.5 dataset as `O3-190`. In v1.5, in order to 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 Core+Rn phases. For example, the "standard" ozone product is a copy of the `O3-240` product. In the case of v1.5 temperature and 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 2.2.

2.4 Forward models used in v1.5

The retrieval algorithms in v1.5 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 line-by-line model that computes radiances on appropriate grids of frequency and tangent pressure that are then convolved with the MLS frequency and angular responses. This is the model that was used to generate a set of simulated radiances for the v1.5 testing.

This model is generally very 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. In the v1.5 retrieval algorithms, its use is restricted mainly to radiance channels whose focus is the upper troposphere and lower stratosphere, as these radiances generally have a non-linear relationship to the state vector.

For many of the MLS channels, a simpler "Linearized" forward model can be used. This 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.

This model is by its nature approximate. Many of the biases and unexpected scatter seen in the v1.5 simulation studies can be attributed to inaccuracies in this model. The model accuracy is a function of the proximity of the retrieved state to the pre-selected state used. The pre-selected states are taken from climatological fields for fixed latitudes and calendar months. In regions where the atmosphere departs dramatically from the climatological values (e.g., in the winter polar vortices), the model will generally be poorer than in other locations, giving rise to stronger biases.

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 for the v1.5 testing, but is not invoked in the v1.5 retrieval algorithms (the handling of clouds is described in more detail in section 2.5).

Table 2.1: The phases that form the v1.5 retrieval algorithms.

Phase	Target species[a]	Measurements	Comment
Init-pTan	T pTan (GHz), GPH	R1A (118 GHz)	Very quick forward model
Update-pTan	T pTan (GHz), GPH	R1A (118 GHz)	Slower more accurate model
Init-UTH	U.T. H_2O	R2 (190 GHz)	
Core+R2A	T, pTan (GHz), GPH, H_2O, N_2O, HNO_3, O_3	R1A (118 GHz), R2 (190 GHz)	H_2O retrieved down to 316 hPa, other species to 215 or 100 hPa, uses costly full forward model.
Core+R2B	T, pTan (GHz), GPH, H_2O, HNO_3, ClO, O_3, HCN, CH_3CN	R1A (118 GHz), R2 (190 GHz)	Main H_2O radiances excluded, products retrieved down to between 316 and 100 hPa. Fast linear forward model used.
High-Cloud	Baseline terms as proxy for cloud contamination	R2 (190 GHz), R3 (240 GHz)	Used for flagging clouds in Core+R3 and later phases, in addition to forming basis for cloud water products.
Core+R3	T, pTan (GHz), GPH, O_3, CO, HNO_3	R1A (118 GHz), R3 (240 GHz)	Retrievals down to 316 hPa
Core+R4A	T, pTan (GHz), GPH, ClO, BrO, HO_2, HOCl, HCl, O_3, HNO_3, CH_3CN	R1A (118 GHz), R4 (640 GHz)	Retrievals down to 147 hPa
Core+R4B	T, pTan (GHz), GPH, N_2O	R1A (118 GHz), R4 (640 GHz)	Retrievals down to 147 hPa
Core+R5	T, pTan (GHz, THz), GPH, OH, O_3	R1A (118 GHz), R5H and R5V (2.5 THz)	Retrievals down to 68 hPa

[a] Tangent pressure and Geopotential height have been abbreviated to pTan (GHz/THz) and GPH respectively. Minor state vector components such as 'baseline' have been omitted.

Table 2.2: The origin of each of the 'standard products' from v1.5

Product	Origin
BrO	Core+R4A (640 GHz)
CH_3CN	Core+R2B (190 GHz)
ClO	Core+R4A (640 GHz)
CO	Core+R3 (240 GHz)
H_2O	Core+R2A (190 GHz)
HCl	Core+R4A (640 GHz)
HCN	Core+R2B (190 GHz)
HNO_3	Core+R3 (240 GHz) at and below 10 hPa, Core+R2A (190 GHz) above
HO_2	Core+R4A (640 GHz)
HOCl	Core+R4A (640 GHz)
N_2O	Core+R4B (640 GHz)
O_3	Core+R3 (240 GHz)
OH	Core+R5 (2.5 THz)
Temperature	Core below 1 hPa, Core+R2A above.

2.5 The handling of clouds in v1.5

Thin clouds and atmospheric aerosols do not affect the MLS measurements as the typical particle sizes are much smaller than the wavelengths of the radiation being observed. However, thick heavy clouds can affect the MLS radiances significantly, mainly through Mie scattering processes. There are two aspects to the handling of clouds in the v1.5 algorithms. The first is the flagging of radiances that are believed to be significantly contaminated by cloud effects. This is done by comparing measured radiances in selected optically thin channels (those that see deepest into the atmosphere) to forward model estimates. Where measured radiances differ significantly from the predictions, cloud contributions to the signal are inferred, and the radiances are flagged as being possibly contaminated. In the early part of the retrieval algorithm, the forward model used for flagging is based on assumptions of 110% relative humidity. Later, further forward model calculations are performed to refine the cloud flags as better information on the actual humidity of the atmosphere is obtained. The retrievals of gas phase species abundances may choose to ignore cloud contaminated radiances, or (in the case of some less impacted channels) to inflate their estimated precision. The other aspect of the cloud handling in v1.5 is the estimation of the ice water content (IWC) within any clouds, based on the MLS radiance observations. This is described in section 3.13.

2.6 Sources of simulated data used to test algorithms

The version 1.5 algorithms have been extensively tested on simulated data. Two sources of such data have been used. The first data are mainly taken from the output of the SLIMCAT model [Chipperfield, 1999], driven by U.K. Met Office temperature and wind data. The data are taken from output of the model on 26 February 1996 (`1996d051`). The model fields were sampled at the locations and times (to the nearest 15 minute time step) of the MLS Level 2 profiles. The model did not produce data for HCN or CH_3CN. The HCN field is taken from a scaling of the CH_4 field (otherwise unused by MLS), while the CH_3CN data is taken from a scaled linear combination of CH_4 and N_2O. For most regions the data above and below the model range are simply tied to the data at the edges of the model. However, for water vapor the tropospheric data are replaced with information from the European Centre for Medium Range Weather Forecasting (ECMWF) scaled by 125%, with the excess over 100% used as a flag to introduce clouds into the model atmosphere. Furthermore, mesospheric temperature, H_2O and O_3 have been modified to introduce more zonal asymmetry.

The second source of simulated data has been generated in a special run of the MOZART model [Park et al., 2004]. These data correspond to a simulated atmosphere for 2 October for an arbitrary year. The data files for this day have been labeled as corresponding to the year 2000 (`2000d276`), though unlike the 1996 data, these data are not representative of the state of the real atmosphere on that date. These data formed part of an intercomparison exercise for all four Aura instruments (the SLIMCAT data were generated purely for use by the MLS team). The model produced files with a 20 minute temporal resolution. These were interpolated to the times and locations of the MLS profiles. As with the SLIMCAT model, no HCN or CH_3CN data were produced. In this case, however, their abundances are assumed to be zero in our simulations rather than being "faked" from other species.

Complete sets of simulated MLS radiances were generated for these days, using the most accurate forward model calculations at our disposal. These formed the basis of all the retrieval simulations shown in the rest of this document.

2.7 A brief note on the `Quality` field

As described in section 1.4, 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 (so 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 v1.5 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 somewhat generously '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 significantly 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.

Chapter 3
Results for 'standard' MLS data products

3.1 Measuring the quality of data products

We report here on results of the quality of MLS retrieval simulations 'closure', meaning how well the retrievals match the 'true' profiles that were used to calculate simulated radiances. However, systematic effects that can arise, for example, from an imperfect forward model, or imperfect calibration/spectroscopy knowledge will not be evident from simulations. Validation and comparisons with correlative data sources (or climatology in some cases) are needed to better evaluate the quality of the v1.5 MLS data. These validations studies are ongoing, but a summary of early results is provided for many of the products. Several of these are discussed in Froidevaux et al. [2005]. Other publications regarding early validation of MLS data are being planned, in addition to results and updates to be provided at Aura validation and other meetings.

The integration, testing and 'tuning' of the v1.5 algorithms involved many test runs of the retrieval software on both the simulated data sets and real MLS observations. Some of the simulation tests used model radiances that had levels of expected instrument noise added to them, others were based on 'clean' radiances (though the retrieval algorithms are still informed of the noise levels to be expected). The quality of these fits is described in a set of "summary" plots for each product. These fall into two broad categories. For the species that show no significant diurnal variation over most of their range, we present a plot that shows in broad latitude bins:

1. the differences from truth (retrieved minus true) and a median bias in the case where noise was included in the simulation,
2. the differences from truth and a median bias in the noise-free case, and
3. the root mean square deviation about the mean bias in the noisy and noise-free cases, along with the RMS of the expected precision reported by the retrieval algorithms.

These are shown both in terms of absolute value (e.g., parts per million) and as a percentage of the mean "true" values in the bins. In each case, the median bias for all the data is shown with a thick black line. The median bias for only profiles where the `Status` field is zero is shown in red. In the case of these simulations, this corresponds to locations and products the retrieval believes to be free from the effects of cloud emission and/or scattering.

The comparison of the expected precision and the observed scatter in the noise-free study tells us how the scatter from 'systematic' problems (errors due to forward model approximations, residual cloud effects, constrained quantities, retrieval 'smoothing' etc.) compares to the scatter we predict from our knowledge of the measurement noise.

The comparison of the estimated precision with the observed scatter in the noisy case is also informative. In the case where there are no significant systematic error sources, and information contributions from the *a priori* and smoothing constraints are small compared to those from the instrument, we would expect the scatter and the precision to agree well. We see that for many products the precision overestimates the scatter by ∼50%. This indicates that the smoothing is having a significant 'calming' effect on the results. The agreement often gets worse at high altitude, indicating that the *a priori* information is also contributing significantly to the results.

For species having both significant diurnal variation (e.g., BrO, ClO, HO_2 and OH), slightly different sets of plots are shown. In these cases it is useful to consider day / night differences when using the MLS data, as this will significantly lessen the impact of many sources of systematic errors in the MLS measurement system. In cases such as BrO in the mid- and lower-stratosphere where it is 'known' that there is insignificant BrO present at night, the day / night difference can be used as a good measure of the actual daytime BrO amount.

To reflect this approach, plots for these species show the differences from truth and median biases in the noise-free cases separately for the ascending half of the Aura orbit (which corresponds to day-time measurements) and the descending half (night-time). Also shown are the differences between the two median biases, which is a good measure of the residual biases to be expected in the day / night differences. Finally, the same scatter and precision summary given for the other species is shown.

As described previously, some products are sufficiently 'noisy' that useful information will not be obtained from single profile observations. In these circumstances, some form of averaging will be required. Accordingly, for BrO, HOCl, HO_2 and OH, the precision and 'scatter' is shown scaled to what would be expected for a monthly (30 day) zonal mean in 5°-wide latitude bins.

3.1.1 A note on comparing to 'true' profiles

As described previously, the MLS retrieved profiles represent a piecewise linear form for the data on fixed pressure tie points (piecewise linear in log vmr for water vapor). These surfaces are spaced at six surfaces per decade change in pressure, thinning out to three above 0.1 hPa. However, the radiances used in our testing were generated by using the full vertical resolution of our 'truth' data of twelve surfaces per decade throughout the atmosphere (though for some products/altitudes there was little or no additional structure at this fine resolution).

In ascertaining the fit to the true profiles achieved by the algorithms, it is necessary to apply the "least squares" smoothing as described in section 1.6. One could choose also to factor in the information in the retrieval averaging kernels as given later in this document. However, for simplicity, we have opted not to do this in our comparisons. Thus our figures show how MLS would compare to an 'ideal' instrument (one whose averaging kernels were the identity matrix).

3.1.2 Overview of species-specific discussion

The remainder of this chapter discusses the quality of each standard product in turn. This is illustrated by a set of plots from the simulation studies, and averaging kernels. Results from preliminary validation studies of real observations are also described. Most importantly, a set of data screening requirements are given, including the useful pressure range, and interpretation of the `Status` and `Quality` fields. There is also discussion of known artifacts, and plans for future versions.

For each product a separate set of plots is shown for the two test data sets (`1996d051` and `2000d276`). While it would be possible to combine the information represented into an 'upper limit' set of plots, it is felt that keeping the information for the two data sets separate conveys a clearer idea to the reader of the quality to be expected from MLS data based on these simulations.

In addition to these "summary" plots, selected horizontal and vertical averaging kernels for each standard product are shown. 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 in horizontal and vertical 'slices'. As these slice integrals do not represent the total area under each kernel, the values shown are not always close to unity. This should not, however, be taken to indicate that the insufficient information derives from the MLS measurements (as would be the inference from more traditional 1D Averaging kernels).

In general we note that the quality of products based on the simulations is often poorer in the winter polar regions where non-linearity effects can be greater. Data quality for some products in the tropical lowermost stratosphere and upper troposphere can be affected by the presence of clouds.

3.2 Bromine monoxide

Swath name: `BrO`

Useful range: 10 – 2.2 hPa

Contact: Nathaniel Livesey, **Email:** `<livesey@mls.jpl.nasa.gov>`

The standard product for BrO is taken from the 640 GHz (Core+R4A) retrievals. 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. Some form of averaging (e.g., monthly zonal means) is required to obtain scientifically useful results.

Simulations

Results from the simulations shown in figures 3.1 and 3.2 indicate that average MLS BrO biases are a few to ten pptv (typical BrO abundances are 5 – 15 pptv). However, taking ascending/descending or day/night differences can reduce such biases to of order 1 – 3 pptv in the upper stratosphere, down to about 10 hPa.

Vertical resolution

Figure 3.3 shows that the vertical resolution for the v1.5 MLS BrO is around 2.5 km.

Early results and validation

The validation of v1.5 BrO is particularly challenging given the low signal to noise of the MLS observations. Studies of monthly mean BrO clearly show biases of order 10 pptv (see figure 3.4). Taking day/night (or ascending/descending) differences can reduce these biases, yielding values that are broadly in line with expectations.

Data screening

Pressure range (10 – 1 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: Day/night or ascending/differences should be considered in any scientific studies to alleviate biases.

Estimated precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: no discernible impact of clouds on the MLS BrO data has been observed, no special attention need be given to profiles flagged as possibly cloudy.

Quality field: Profiles with a value of the `Quality` field (see section 1.4) less than 1.0 should not be used. This flag is an indication of poor radiance fits; a very small fraction of BrO profiles (much less than 1%) will be discarded via this screening.

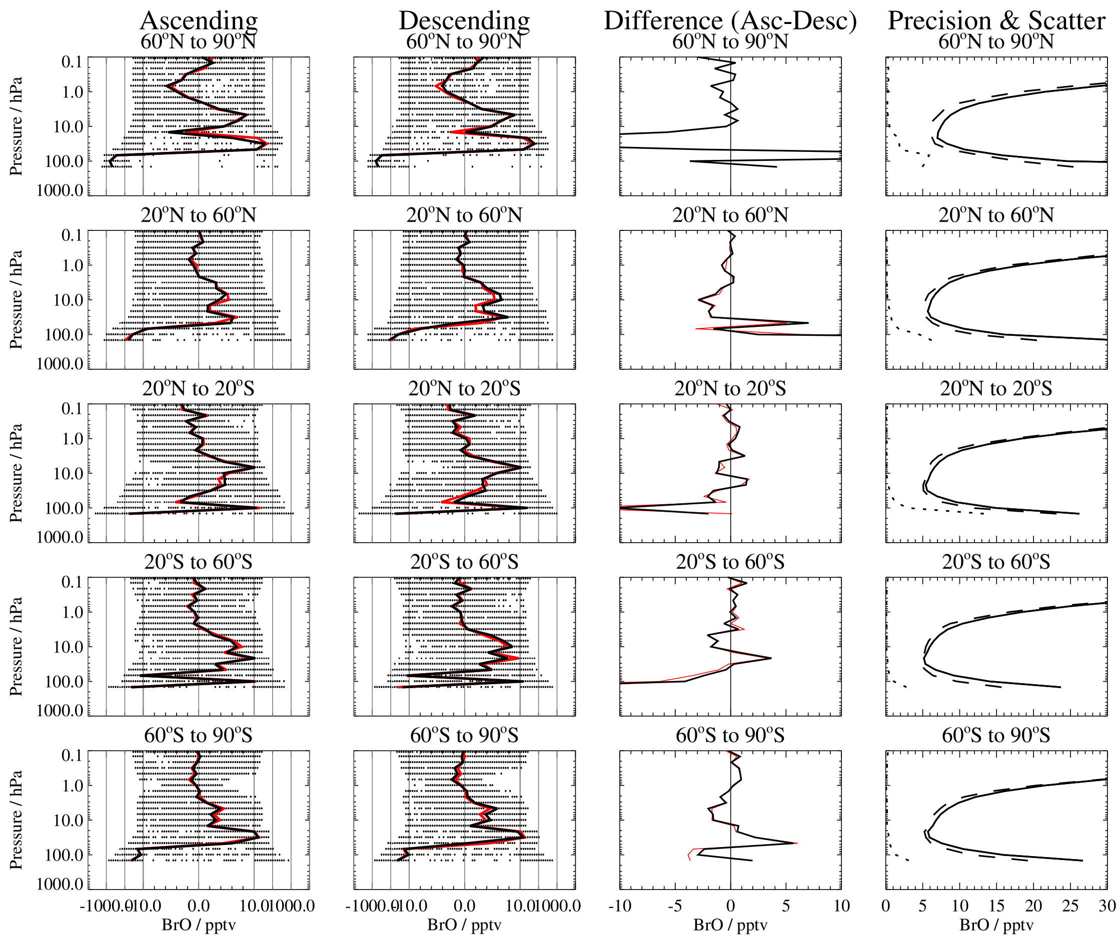


Figure 3.1: A summary of the v1.5 data quality for BrO for the `1996d051` test dataset. Each row of panels represents a broad latitude bin. The first two columns show, for the noise-free case, the differences between the retrieved and true BrO as a function of pressure for the ascending and descending phases of the Aura orbit (corresponding to mainly day and mainly night observations respectively). Also shown is a solid line that indicates the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the difference in the median biases (solid black lines in previous columns) between the ascending and descending side. The fourth column shows the mean estimated precision of monthly zonal means of BrO in 5° wide latitude bins (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases, scaled to correspond to the 'scatter' that would be expected in the monthly zonal means. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

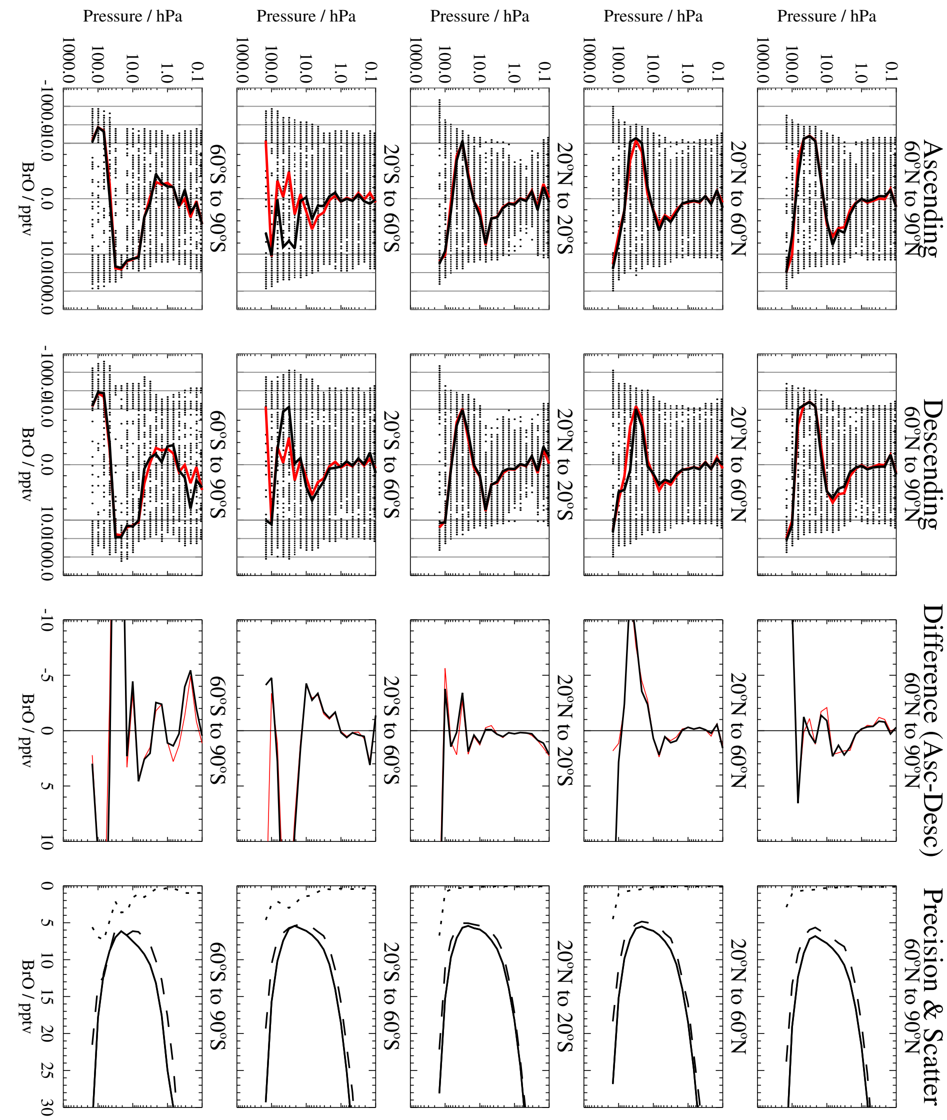


Figure 3.2: A summary of v1.5 data quality for BrO as figure 3.1 for the 2000d276 test data set.

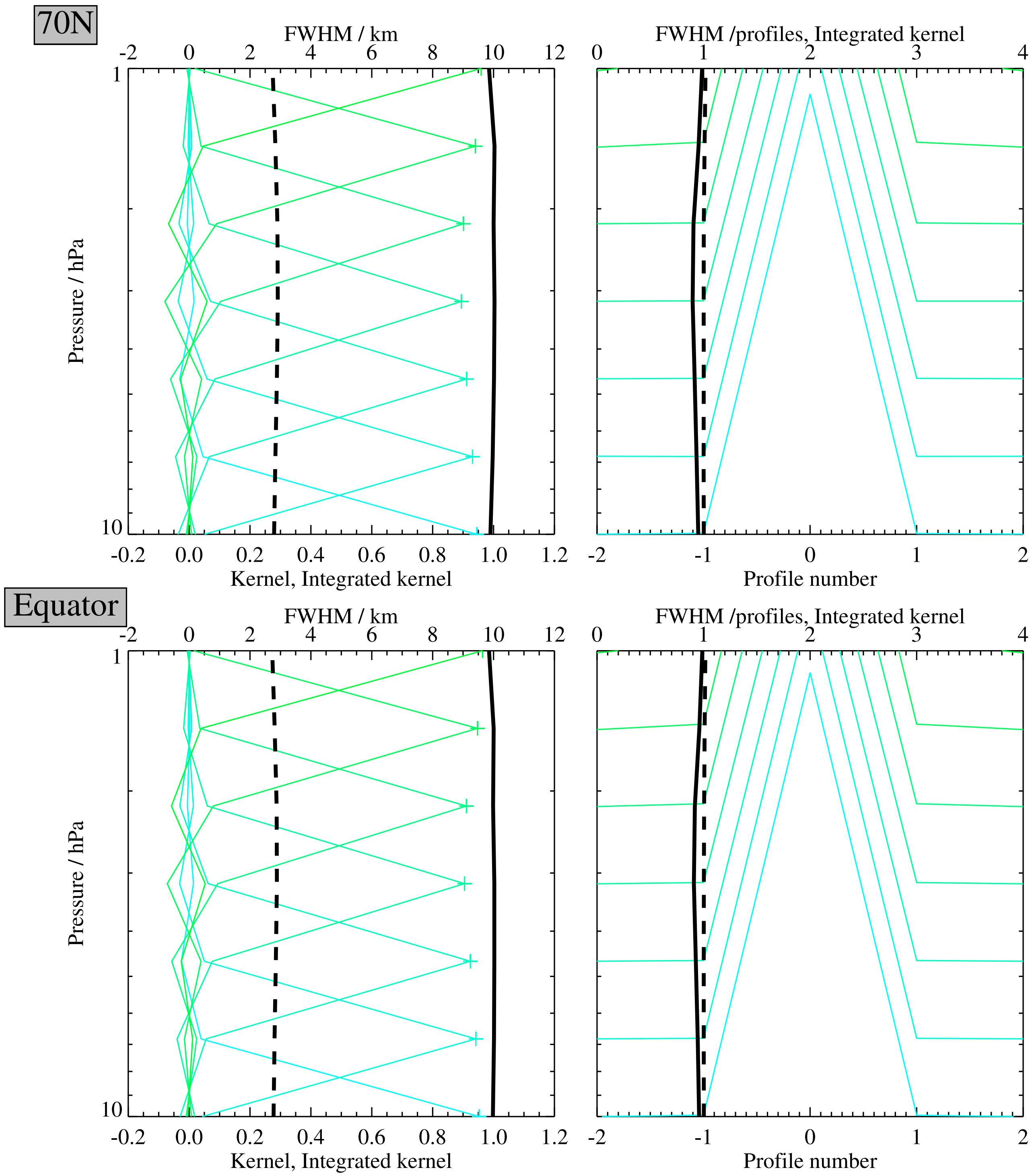


Figure 3.3: The left hand plots show the vertical averaging kernel for BrO for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

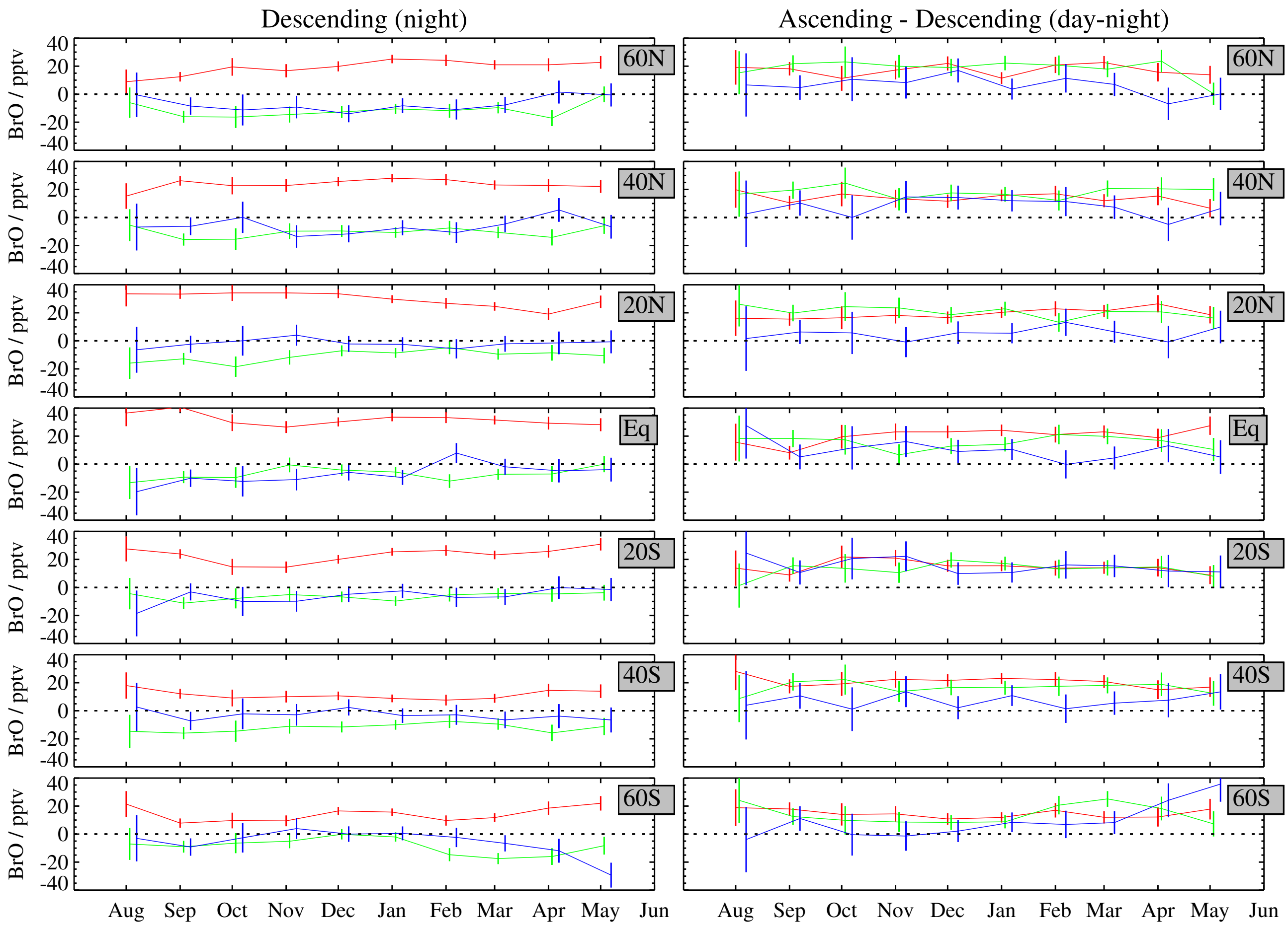


Figure 3.4: The left hand plots show monthly averaged night time BrO for 10 hPa (red), 4.6 hPa (green), and 2.2 hPa (blue) for all the v1.5 data processed from August 2004 to June 2005. Expected abundances of BrO at night are essentially zero at these heights. Values therefore indicate a combination of noise and biases. The error bars are the 1σ uncertainty in the means, as expected from precision. Probable biases as high as $\sim$20 pptv are seen, with $\sim$20 pptv variability. The right hand column shows day/night differences which are taken to represent the daytime abundance. More temporal stability is seen once these differences are taken. It is vital to consider these differences rather than just daytime BrO in scientific studies.

Artifacts

- Significant biases are seen in the BrO data, as discussed above. Day/night (or ascending/descending) differences must be used to reduce these.

Priorities for future versions

- Future data processing versions may introduce more vertical and horizontal smoothing for the BrO retrievals. The consequent gain in precision is felt to be more advantageous than a drop in vertical resolution from 3 to 6 km.

- Improvements will be sought in the stability of the BrO biases.

- Future versions will also seek to improve the quality of the BrO observations in the mid- and lower stratosphere.

3.3 Methyl cyanide

Swath name: `CH3CN`

Useful range: To be determined.

Contact: Nathaniel Livesey, **Email:** <livesey@mls.jpl.nasa.gov>

The standard methyl cyanide product is taken from the 190 GHz (Core+R2A) retrieval.

Simulations

The simulation results shown in figures 3.5 and 3.6 show that significant biases of several tens of pptv are to be expected in v1.5 CH_3CN observations, being worst at pressures greater than $\sim$46 hPa. The noise in individual profiles is such that daily zonal means or similar averages are required for useful scientific study.

Vertical resolution

The averaging kernels in figure 3.7 indicate that the vertical resolution of v1.5 CH_3CN is around 6 km in the lower stratosphere, worsening to about 10 km in the upper stratosphere.

Early results and validation

Early studies indicate that CH_3CN should be considered a research product in v1.5. Values of order 100 – 150 pptv are seen, significantly higher than the abundances expected. These biases are likely to be due to known problems in v1.5 fitting the radiance signals in the region of the weak CH_3CN emission. The data also show significant unrealistic variability, well above the levels of noise expected, in the lowermost stratosphere and upper troposphere, where it is hoped that useful study can be made of enhancement 'events' [Livesey et al., 2004]. This variability currently hampers scientific study of such events.

Data screening

Do not use: The v1.5 standard product CH_3CN data should not be used without significant discussion with the MLS science team.

Artifacts

As described above, significant biases are seen at all levels, and unrealistic levels of variability are seen in the lower stratosphere and upper troposphere.

Priorities for future versions

Future versions should improve the modeling of MLS radiance signals in the CH_3CN spectral region, leading to improvements in this product.

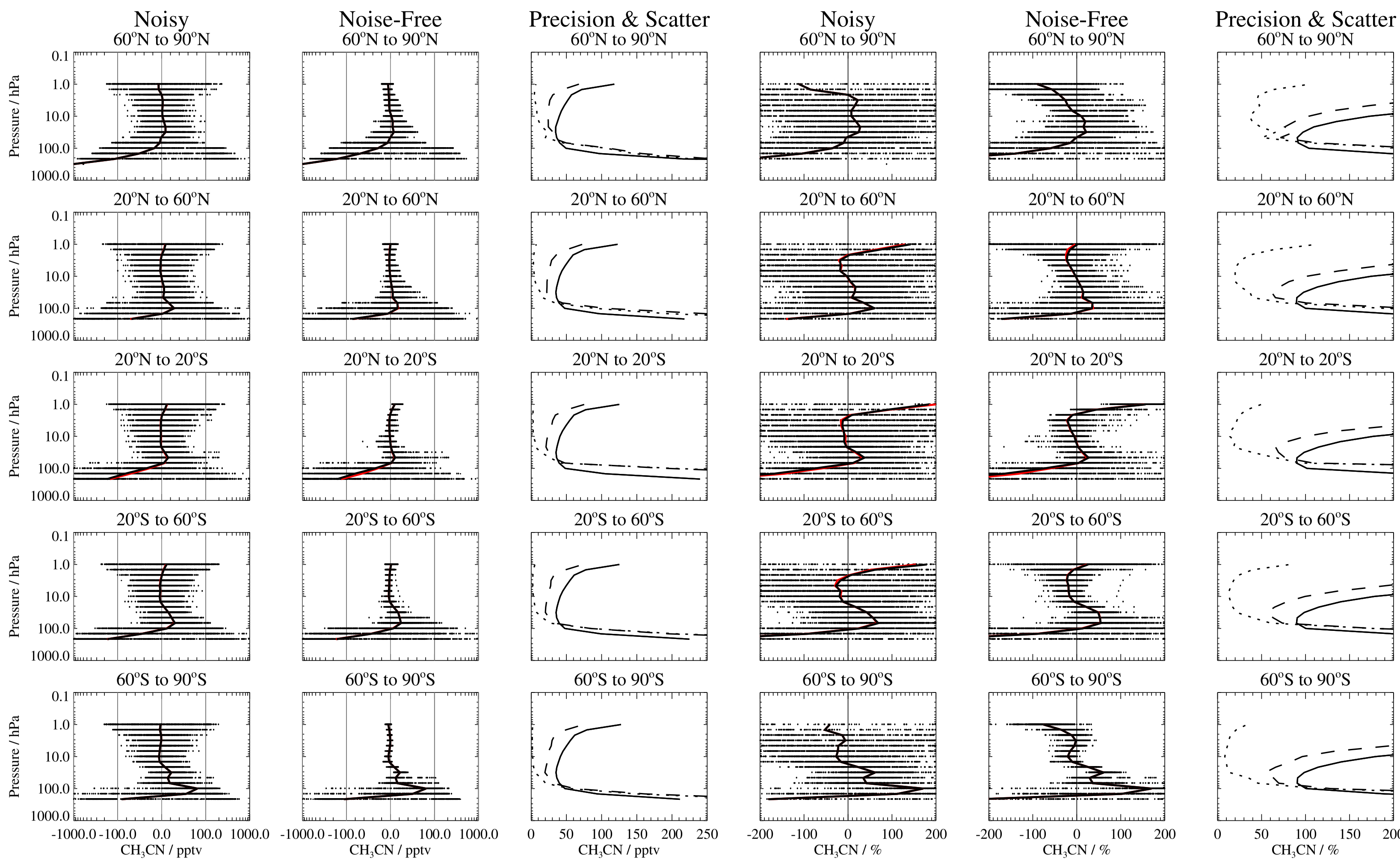


Figure 3.5: A summary of the v1.5 data quality for CH_3CN for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true CH_3CN as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of CH_3CN (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

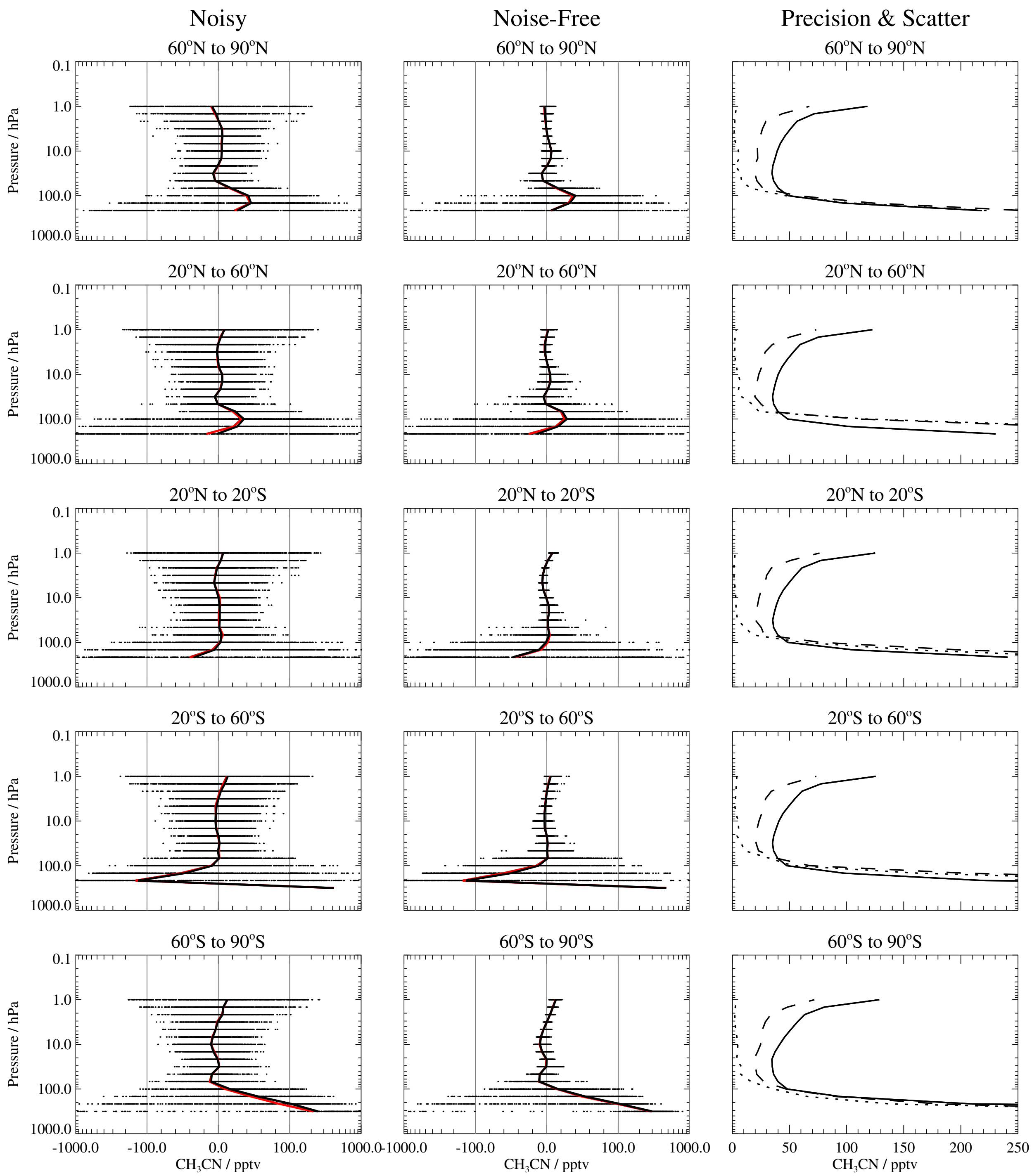


Figure 3.6: A summary of v1.5 data quality for CH_3CN similar to figure 3.5 except for the `2000d276` test data set. The percentage plots are omitted here as the 'true' values are zero.

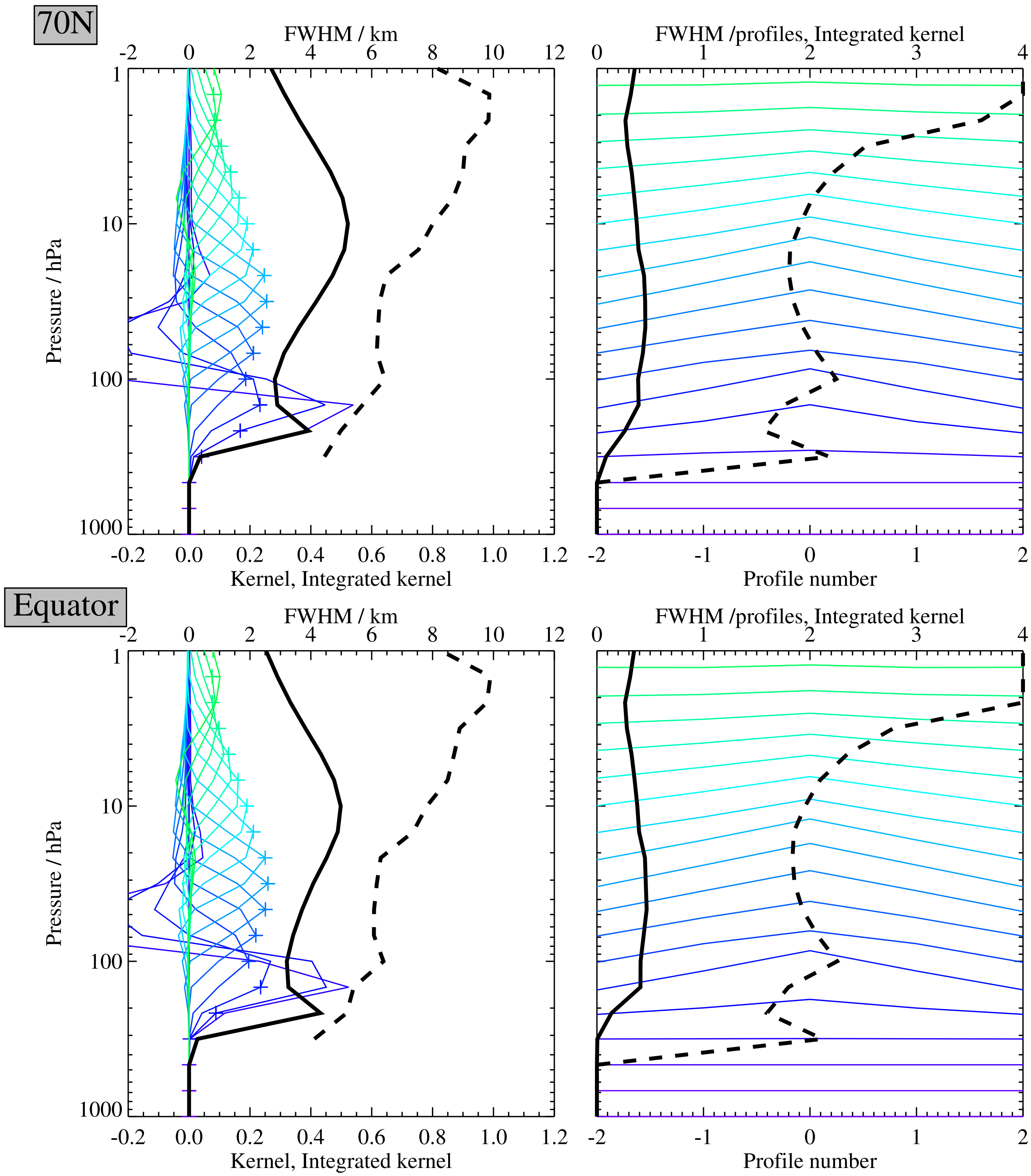


Figure 3.7: The left hand plots show the vertical averaging kernel for CH_3CN for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

3.4 Chlorine monoxide

Swath name: `ClO`

Useful range: 100 – 1 hPa

Vertical resolution: 3 to 5 km

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

The standard product for ClO is taken from the 640 GHz (Core+R4A) retrieval.

Simulations

ClO is strongly diurnal in the lower stratosphere; day-night differences can be used to reduce systematic effects in the measurements from 100 to 10 hPa. Simulations (see Figures 3.8 and 3.9) show residual average biases in these differences (indicating systematic errors that cannot be eliminated by taking day-night differences) as large as 0.1 ppbv in the winter polar regions. Elsewhere, residual average biases are less than 0.01 ppbv (often considerably so).

Vertical resolution

Based on Figure 3.10, the ClO vertical resolution varies with altitude, from ~3 km over the range 100 to 10 hPa to ~5 km near the top of the profile.

Early results and validation

The estimated single-profile precision reported by the Level 2 software varies from ~0.15 to ~0.2 ppbv over the range 100 to 10 hPa, degrading to 0.4–0.5 ppbv near 1 hPa. The observed scatter in the data, evaluated in a 20°-wide latitude band centered around the equator where natural variability is expected to be small in the lower stratosphere, suggests a measurement precision of 0.1–0.2 ppbv throughout the profile. Comparisons with correlative data sources have not yet been undertaken for ClO, so accuracy estimates are not available. However, time series of daytime, nighttime, and day-night difference values from almost nine months of version 1.5 data, for both the `ClO-640` and `ClO-190` data products, have been examined in 5°-wide equivalent latitude bands between 87.5°S and 87.5°N on the 660, 580, 520, 460, and 410 K potential temperature surfaces (corresponding to pressure levels of 22, 32, 46, 68, and 100 hPa, respectively). At the topmost level, nighttime mixing ratios are approximately zero at all equivalent latitudes and seasons for both ClO products. At the lower levels, however, a persistent negative bias of as much as ~0.3 ppbv is evident at low and middle latitudes in both daytime and nighttime mixing ratios from the `ClO-640` retrievals; no such bias appears to be present in the `ClO-190` data. At polar latitudes, the `ClO-640` nighttime mixing ratios temporarily exhibit nonnegligible positive values during the winter when ClO is enhanced; at other seasons a negative bias comparable to that always present at low and middle latitudes is seen. This change in behavior in the winter high latitudes is largely absent in the `ClO-190` data, suggesting that for the most part it does not arise from physical processes. Taking day-night differences in the lower stratosphere effectively eliminates the negative bias; it also leads to reduced ClO mixing ratios during the winter enhancement at polar latitudes, since nighttime values are slightly positive at that time/location. Because the systematic negative bias in the MLS ClO standard product can be as large as ~0.3 ppbv at the lowest retrieval levels, it is recommended that day-night differences be taken in studies for which knowledge of the lower stratospheric ClO mixing ratios to better than ~0.3 ppbv is needed.

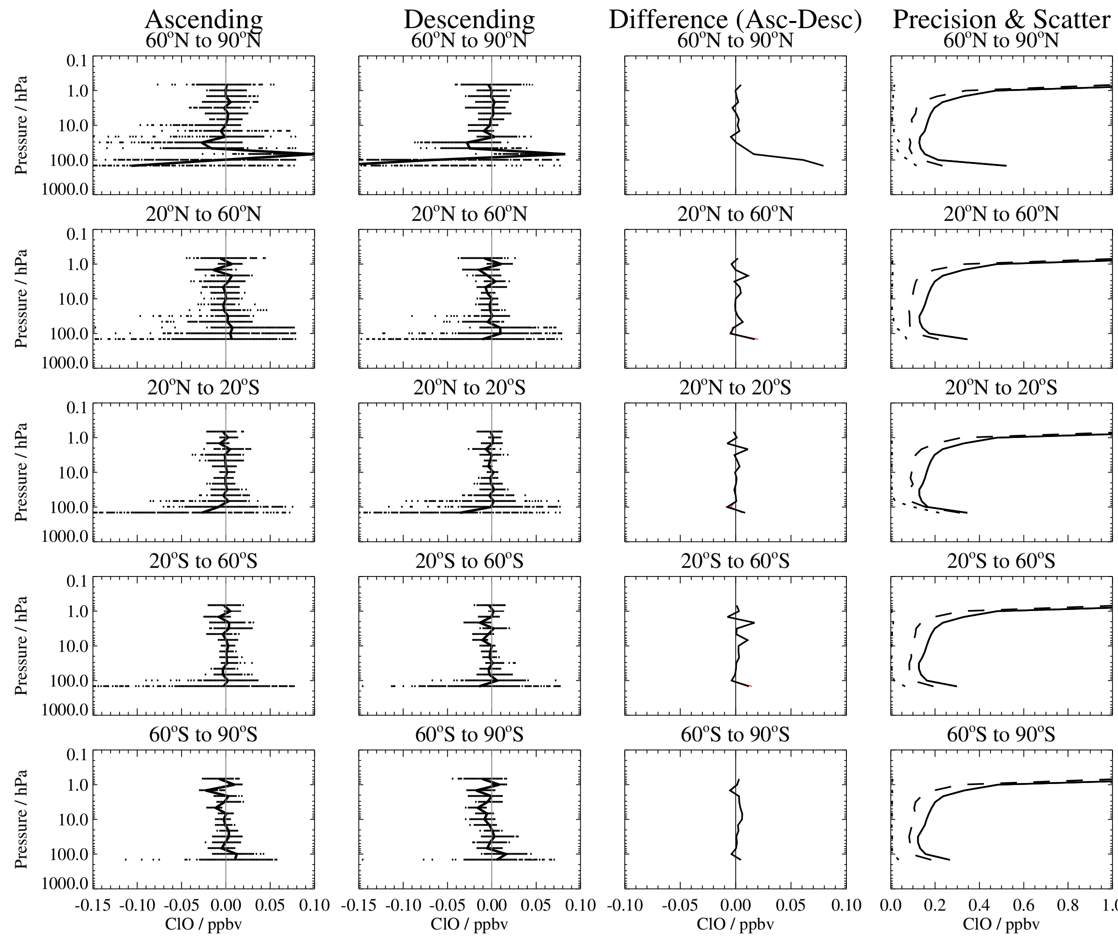


Figure 3.8: A summary of the v1.5 data quality for ClO for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show, for the noise-free case, the differences between the retrieved and true ClO as a function of pressure for the ascending and descending phases of the Aura orbit (corresponding to mainly day and mainly night observations, respectively). Also shown is a solid line that indicates the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the difference in the median biases (solid black lines in previous columns) between the ascending and descending side. The fourth column shows the mean estimated precision of individual ClO profiles (solid line), and the rms scatter about the mean bias seen in the noisy (dashed line) and noise-free (dotted line) cases.

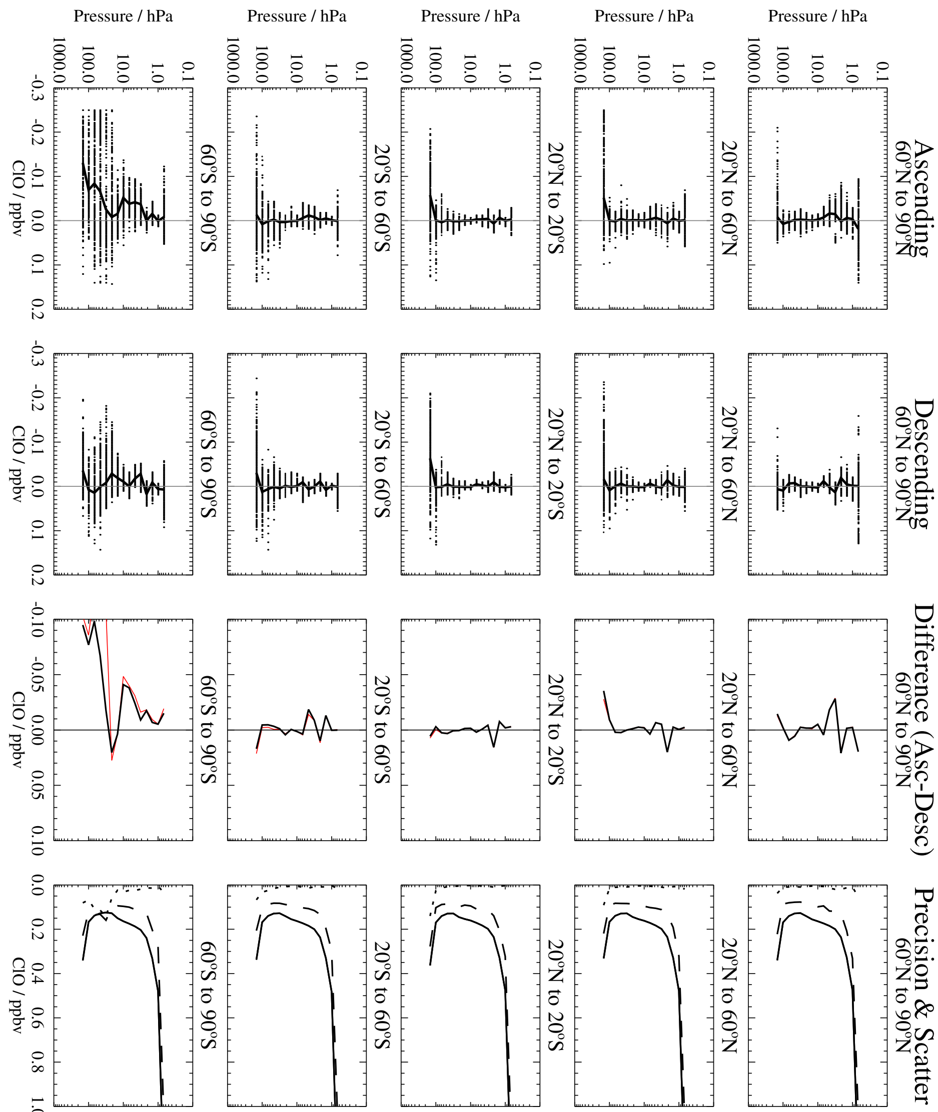


Figure 3.9: A summary of v.5 data quality for ClO as figure 3.8 for the 2000d276 test data set.

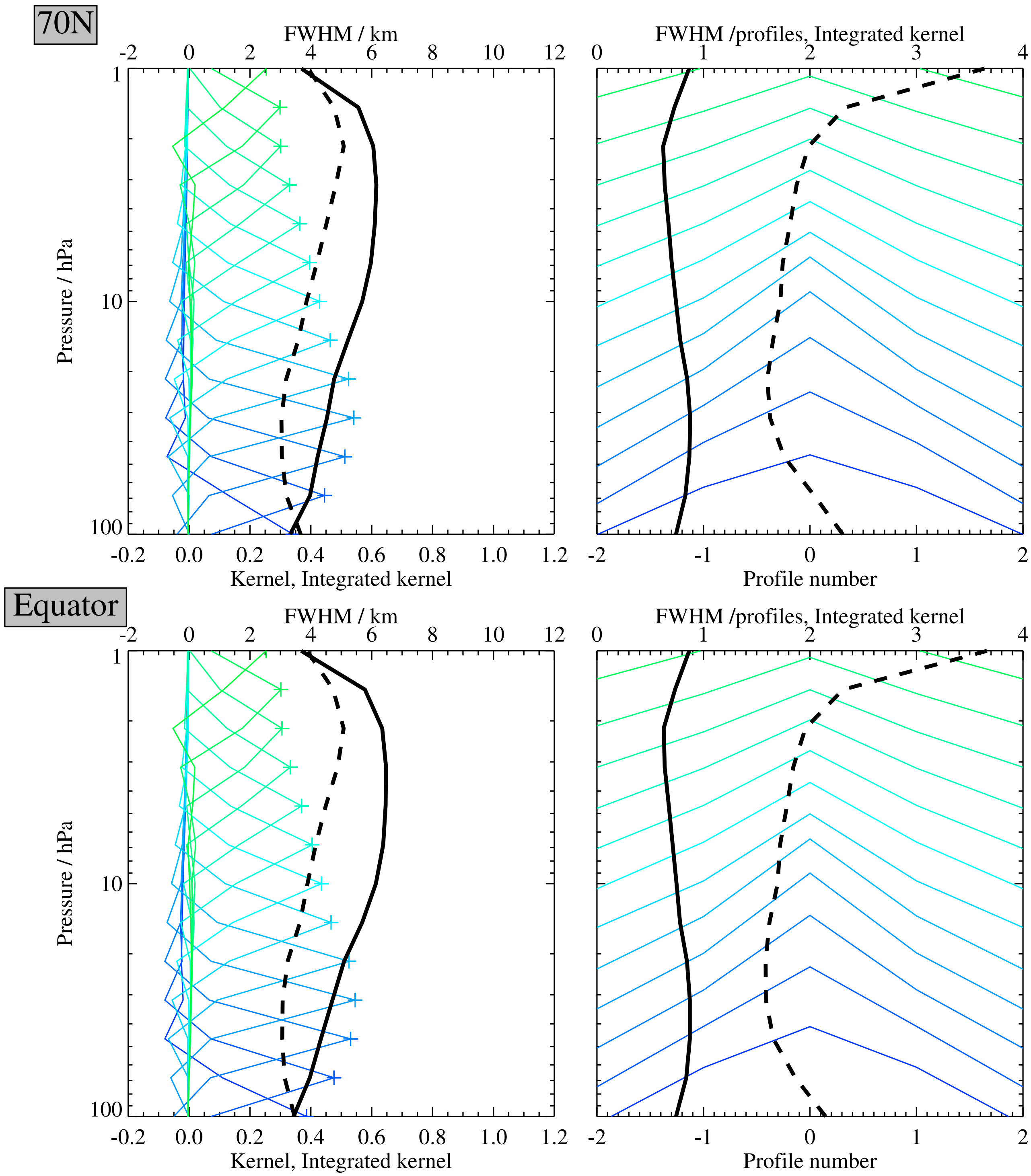


Figure 3.10: The left hand plots show the vertical averaging kernel for ClO for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

Data screening

Pressure range (100 – 1 hPa): Values outside this range are not recommended for scientific use.

Diurnal differences: Day/night or ascending/descending differences will be required in the lower stratosphere if accuracies of better than ∼0.3 ppbv are required.

Estimated precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: An examination of several months of v1.5 data indicates that clouds do not have a significant impact (outside the noise) on ClO profiles down to 100 hPa; there is currently no apparent need to discard profiles or profile portions where `Status` values indicate the existence/influence of clouds (see section 1.4).

Quality field: MLS ClO profiles typically have high `Quality` values (see section 1.4), indicating generally good radiance fits. Imposing a threshold value of 2.7 for ClO `Quality` (below which a profile is discarded) throws out about 1% of data, eliminating profiles with obvious `Quality` outliers while minimizing rejection of profiles with apparently decent fits.

Artifacts

A persistent negative bias of as much as 0.3 ppbv is seen at all latitudes and seasons (outside of the winter polar regions, as discussed above) at the lowest retrieval levels (below about 32 hPa); taking day-night differences effectively eliminates this negative bias.

Priorities for future data version(s)

- Reduce the persistent negative bias in the ClO mixing ratios at the lowest retrieval levels.
- Attempt to improve the retrievals at 147 hPa.

3.5 Carbon monoxide

Swath name: CO

Useful range: 215 – 0.0046 hPa

Vertical resolution: 4.5 to 6 km

Contact: Mark Filipiak, **Email:** <M.J.Filipiak@ed.ac.uk>

The standard product for version 1.5 CO is taken from the 240 GHz (Core+R3) retrieval.

Simulations

Simulations (see Figures 3.11 and 3.12) indicate good closure for CO in the stratosphere and upper troposphere, typically to better than ∼20 ppbv. There is large scatter in the upper troposphere, and there are oscillations in the mesosphere. In the winter upper stratosphere, where CO-rich air has descended from the mesosphere/thermosphere, large biases and scatter are seen.

Vertical resolution

Based on Figure 3.13, the vertical resolution for CO is ∼4.5 km in the upper troposphere and lower stratosphere, and degrades to 6 km in the upper mesosphere. Averaging is required for measurements of background concentrations. Enhanced mixing ratios from biomass burning or industrial emissions are measurable using individual profiles.

In the stratosphere the mixing ratios of CO are very low (∼20 ppbv) and measurements require averaging. In the upper stratosphere and lower mesosphere, descent of mesospheric air (CO mixing ratios ∼100 – 1000 ppbv) into the winter polar vortex is measurable in individual profiles.

Early results and validation

Comparisons with ACE data [Froidevaux et al., 2005] indicate that the MLS CO data have a positive bias of 5% in the mid-stratosphere (but see Artifacts below), increasing to 50 – 100% in the mesosphere and thermosphere. Comparisons with aircraft (AVE) and balloon (ALIAS, Mark-IV) data indicate that the MLS CO data have a positive bias at 215 hPa; values at this level are also generally 2× larger than those from GEOS-CHEM model simulations.

Data screening

Pressure range (215 – 0.0046 hPa) Values outside this range are not recommended for scientific use.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number (bit '0' set) should not be used. Data in the troposphere should not be used if the data are marked 'questionable' (`Status` bit 1 set), this signals profiles affected by clouds; data at pressures smaller than 100 hPa can still be used in this case (see section 1.4.)

Quality field: Profiles with a value of the **Quality** field (see section 1.4) less than 0.05 should not be used, this is an indication of poor radiance fits, even for reasonable-looking profiles. A very small fraction of CO profiles (much less than 1%) will be discarded via this screening.

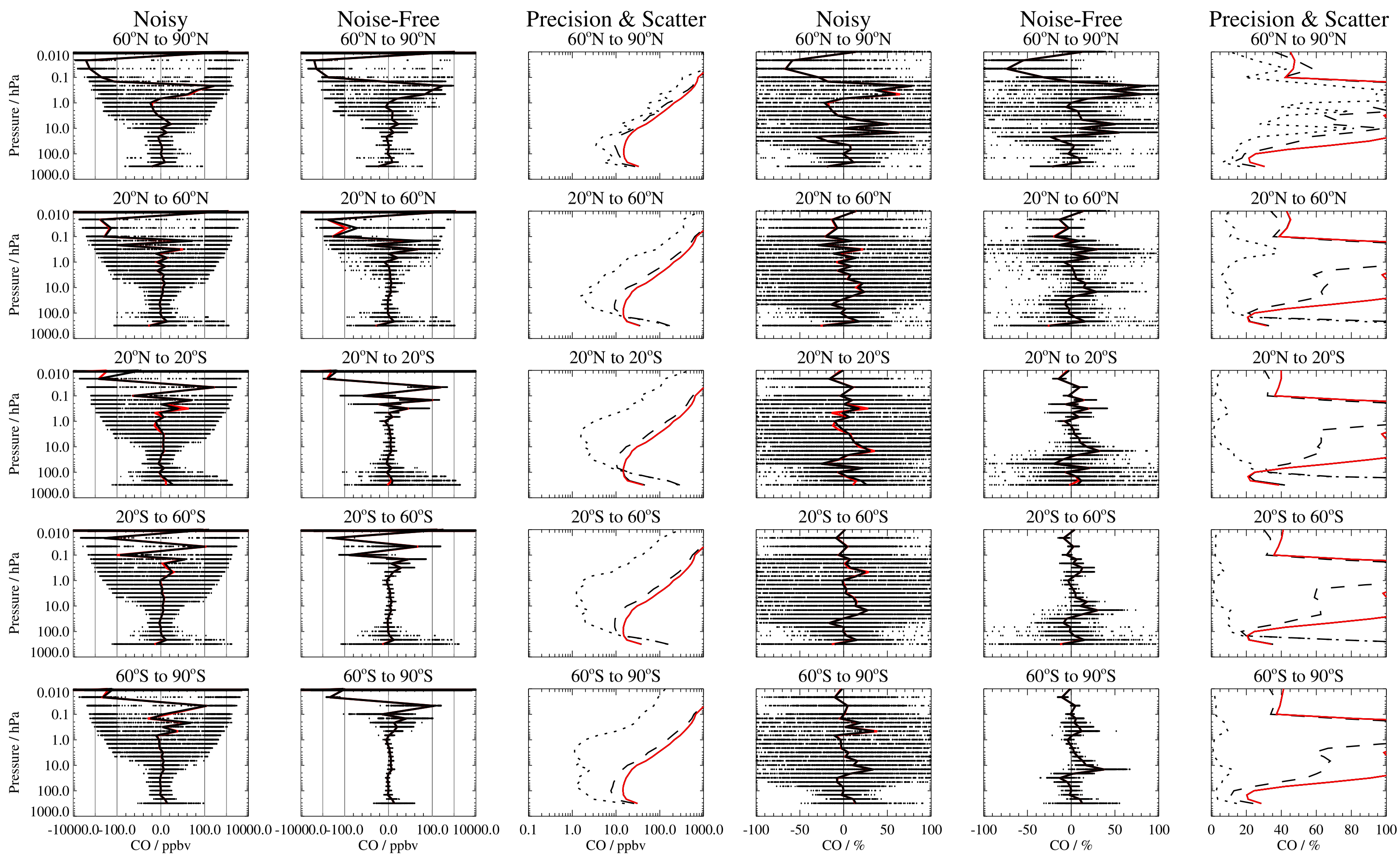


Figure 3.11: A summary of the v1.5 data quality for CO for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true CO as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of CO (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

CO

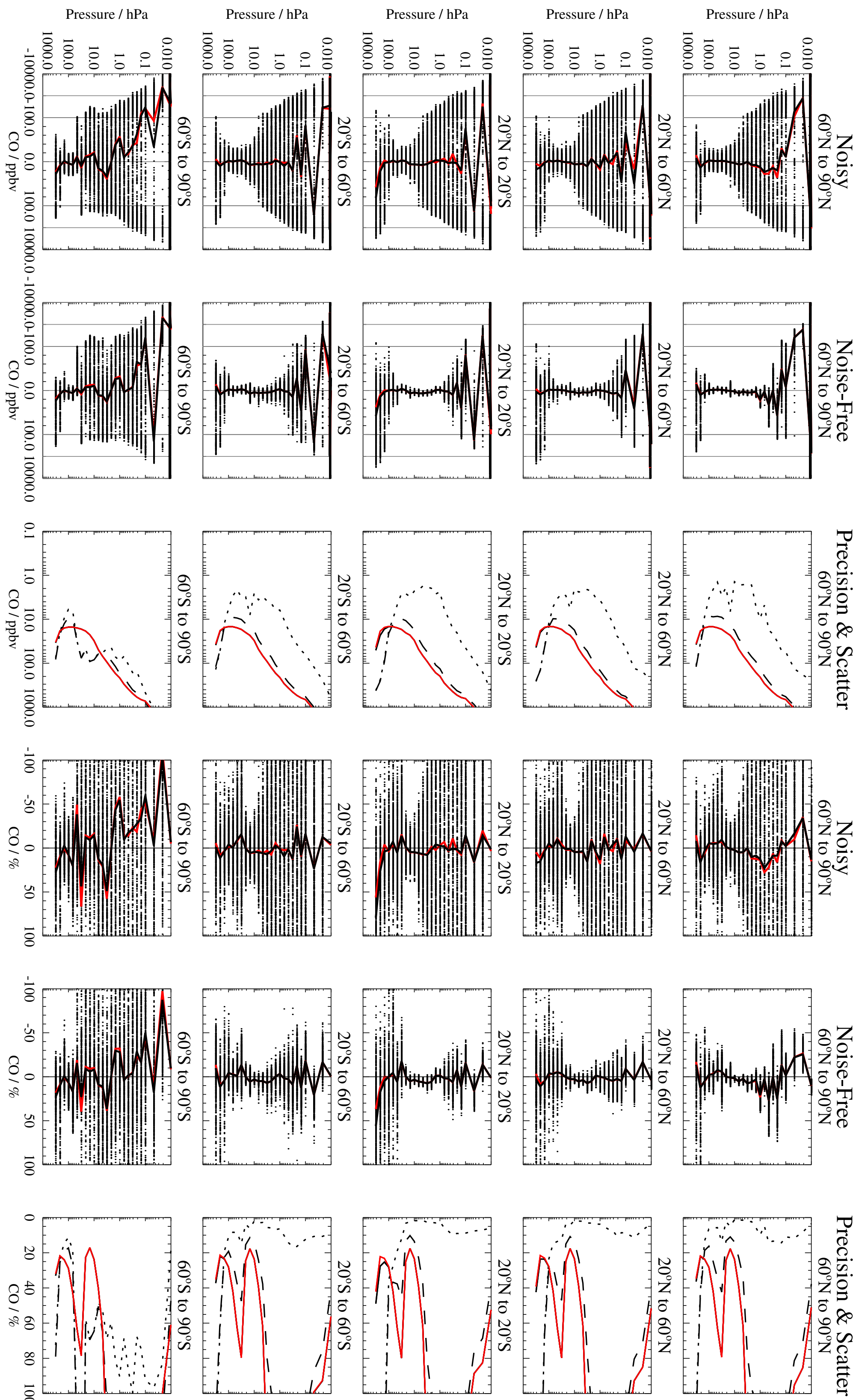


Figure 3.12: A summary of v1.5 data quality for CO as figure 3.11 for the 2000d276 test data set.

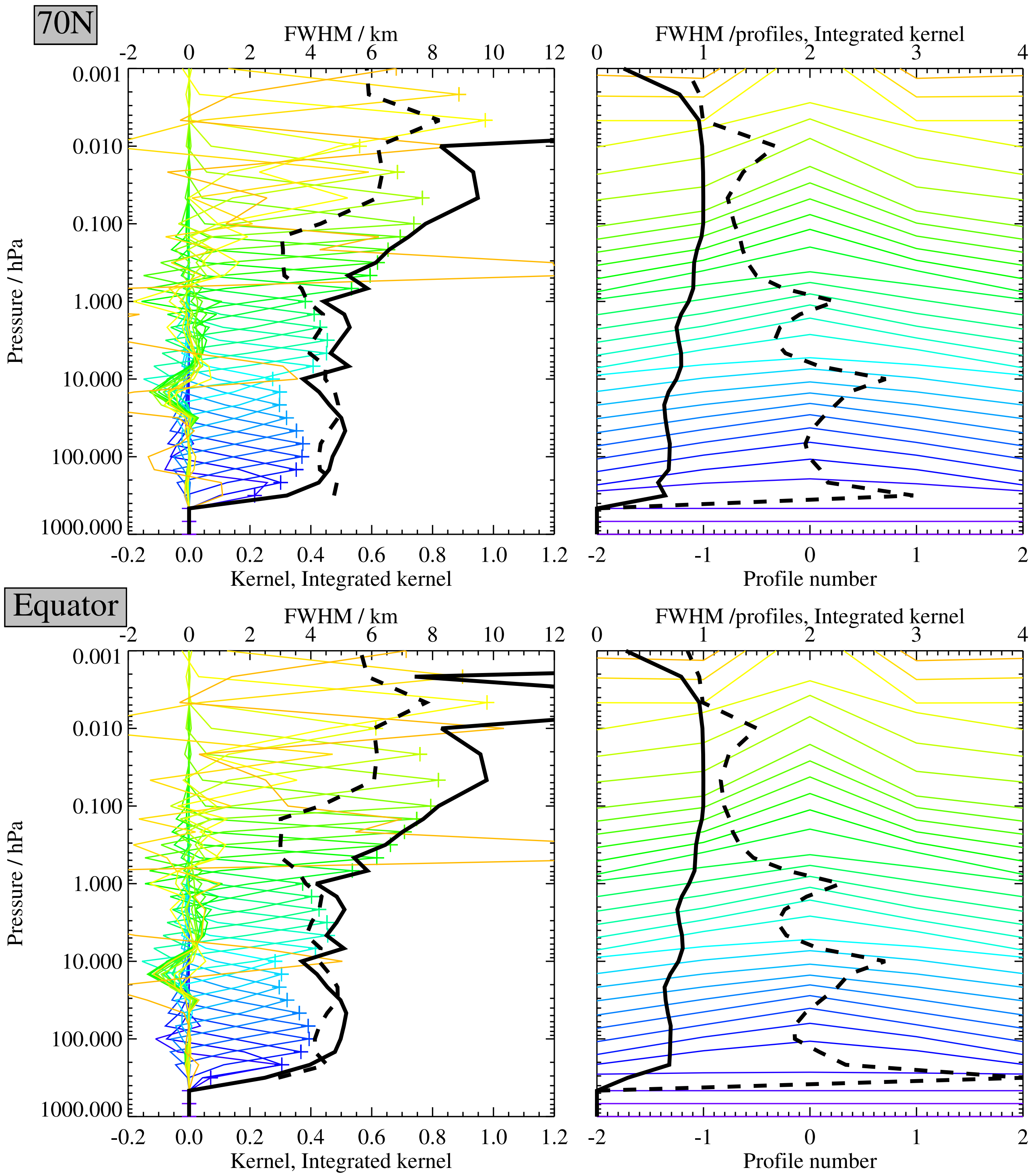


Figure 3.13: The left hand plots show the vertical averaging kernel for CO for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

CO

Artifacts

- There are large, persistent vertical oscillations in the upper stratosphere and mesosphere. These can be seen in Figures 3.11 and 3.12 and are also apparent in comparisons with ACE correlative data. The oscillations have similar magnitude to the estimated precision and appear to be a result of insufficient smoothing in the v1.5 retrievals.
- There is a small ($\sim$10 ppbv) positive bias in the mid- to upper-stratosphere, but values near 30 hPa in the tropics, 215 hPa at high latitudes, are negative (~ -10 ppbv). At these heights the mixing ratio of CO has a minimum in other datasets.
- The CO retrieval at 68 – 32 hPa at high latitudes appears to be affected by the large mixing ratios of nitric acid (HNO_3) found in these regions: there is a correlation between the fields, seen in maps and in scatter plots. There does not appear to be any dynamical or chemical reason for these correlations and there are weak HNO_3 lines in the frequency band used to measure CO so it is likely that there is a problem with the retrieval; the cause is still being investigated.
- Values at 215 hPa have a large positive bias and/or scaling ($\sim 2\times$ larger than values from the GEOS-CHEM model).

Priorities for future data version(s)

- Improve the upper tropospheric data: correct the bias at 215 hPa, reduce the scatter, and extend the useful range to 316 hPa, if possible.
- Remove the HNO_3 contamination at high latitudes.
- Remove the vertical oscillations in the mesosphere.

3.6 Geopotential height

Swath name: GPH

Useful range: 316 – 0.001 hPa

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

The standard product for GPH is formed from the retrieval of a reference geopotential height for the 100 hPa surface and a hydrostatic integration of the standard product temperature profiles.

GPH

Simulations

In simulations of GPH retrievals, biases in the troposphere and stratosphere are less than 50 m except in the uppermost stratosphere (1.47 – 1.0 hPa) in the 1996d051 simulation, where they are less than 150 m. In the mesosphere and lower thermosphere (1 – 0.001 hPa) the 2000d276 simulation shows biases less than 150 m at latitudes 60°S – 60°N and less than 300 m in the polar bins. The 1996d051 simulation is more poorly behaved. At 60°S – 90°S there is a negative 500 m bias at 0.1 hPa and a positive 500 m bias at 0.001 hPa. At 60°N – 90°N there is a positive 120 m bias at 0.32 hPa which trends to a 950 m bias at 0.001 hPa.

Early results and validation

Comparisons of MLS GPH with the GMAO GEOS-4 model values show MLS values to be higher by 0 – 300 m at the 100 hPa reference level. The largest differences are in the winter pole and the smallest are in the ascending equator crossings. The warm bias in MLS stratospheric temperatures relative to GEOS-4 is reflected in increasingly positive MLS GPH biases relative to GEOS-4 through the stratosphere: 100 – 500 m at 10 hPa and 100 – 600 m at 1 hPa. Estimated precision of GPH at the 100 hPa reference level is typically 27 m at 316 hPa, 14 m at 100 hPa, 23 m at 10 hPa, 29 m at 1 hPa, 39 m at 0.1 hPa, 50-60 m at 0.01 hPa and 70-85 m at 0.001 hPa.

GPH precision

The GPH standard-product precision field is not being correctly written to the v01.51 data files. When needed, it may be calculated from the reference GPH precision from the core phase (L2gpPrecision in the refGPH-Core swath in the DGG file) and the standard temperature precision. The precision of the 100 hPa surface of the standard GPH is taken from the refGPH precision. The uncertainty in the incremental GPH between adjacent retrieval levels is the product of the slab-averaged uncertainty of the temperature, the thickness of the slab in dimensionless units of $z = -\log(P/1\text{hPa})$ and $\kappa = 67.4018\,\text{m/K}$. The value of κ, which scales height to temperature with a combination of the gas constant, the molar-mass of air and a constant acceleration (approximately the earth surface gravity at 45° latitude), is adjusted above $z = 2.5$ to account for decreasing molar mass of air at high altitudes.

Thus, for surfaces (index j) below the 100 hPa reference level, the geopotential height precision (σ^{GPH}) is given by

$$\sigma_j^{\text{GPH}} = \left[\left(\sigma^{\text{ref}}\right)^2 + \frac{1}{2} \sum_{i=j}^{6} (\kappa_i \sigma_i^{\text{T}} + \kappa_{i+1} \sigma_{i+1}^{\text{T}})(z_{i+1} - z_i) \right]^{\frac{1}{2}}, \tag{3.1}$$

and for surfaces (index j) above the 100 hPa reference level,

$$\sigma_j^{\text{GPH}} = \left[\left(\sigma^{\text{ref}}\right)^2 + \frac{1}{2} \sum_{i=8}^{j} (\kappa_i \sigma_i^{\text{T}} + \kappa_{i-1} \sigma_{i-1}^{\text{T}})(z_i - z_{i-1}) \right]^{\frac{1}{2}} \tag{3.2}$$

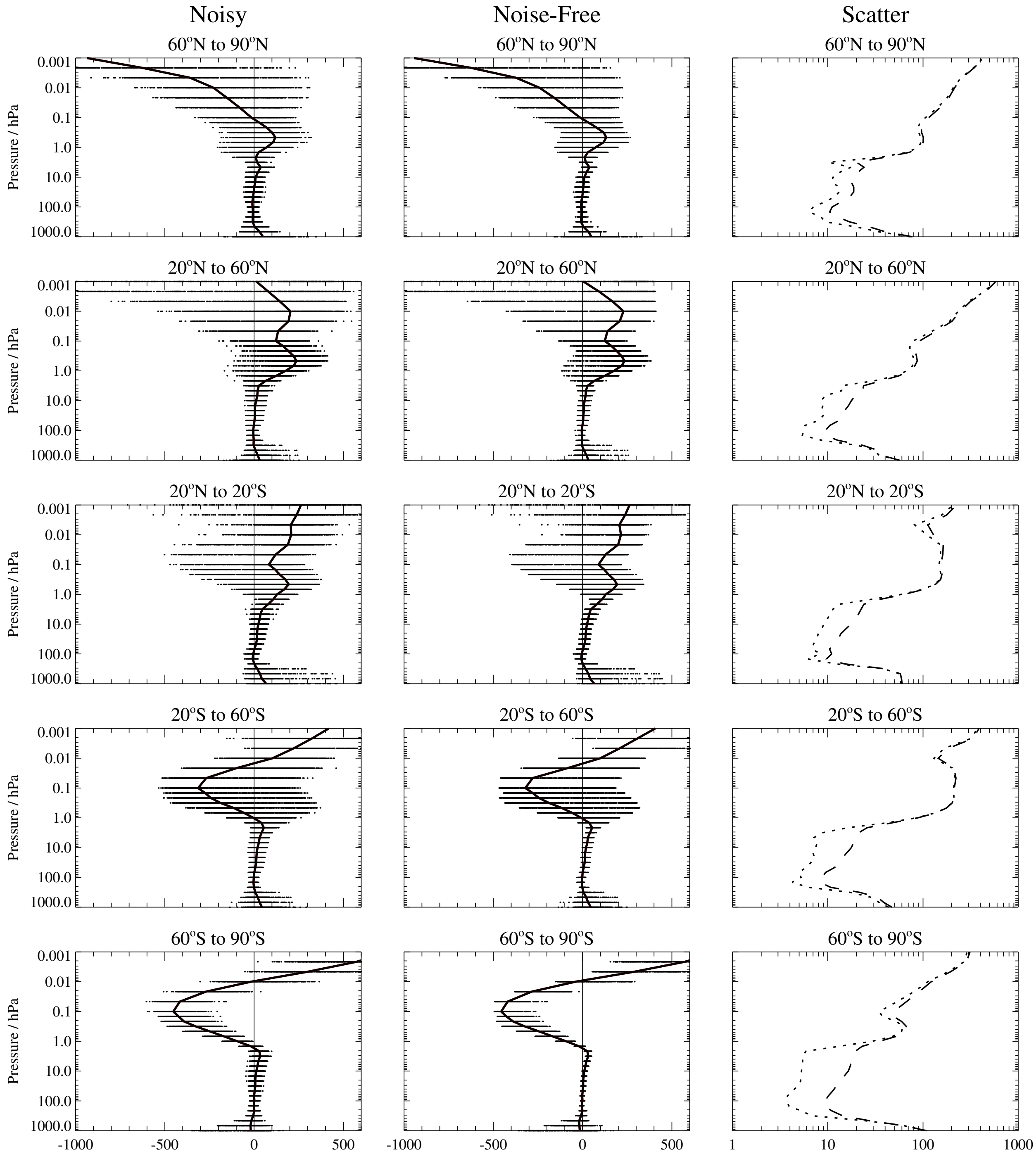


Figure 3.14: A summary of the v1.5 data quality for GPH for the `1996d051` test dataset. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved GPH and the true GPH as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The final column shows the mean estimated precision of GPH (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases.

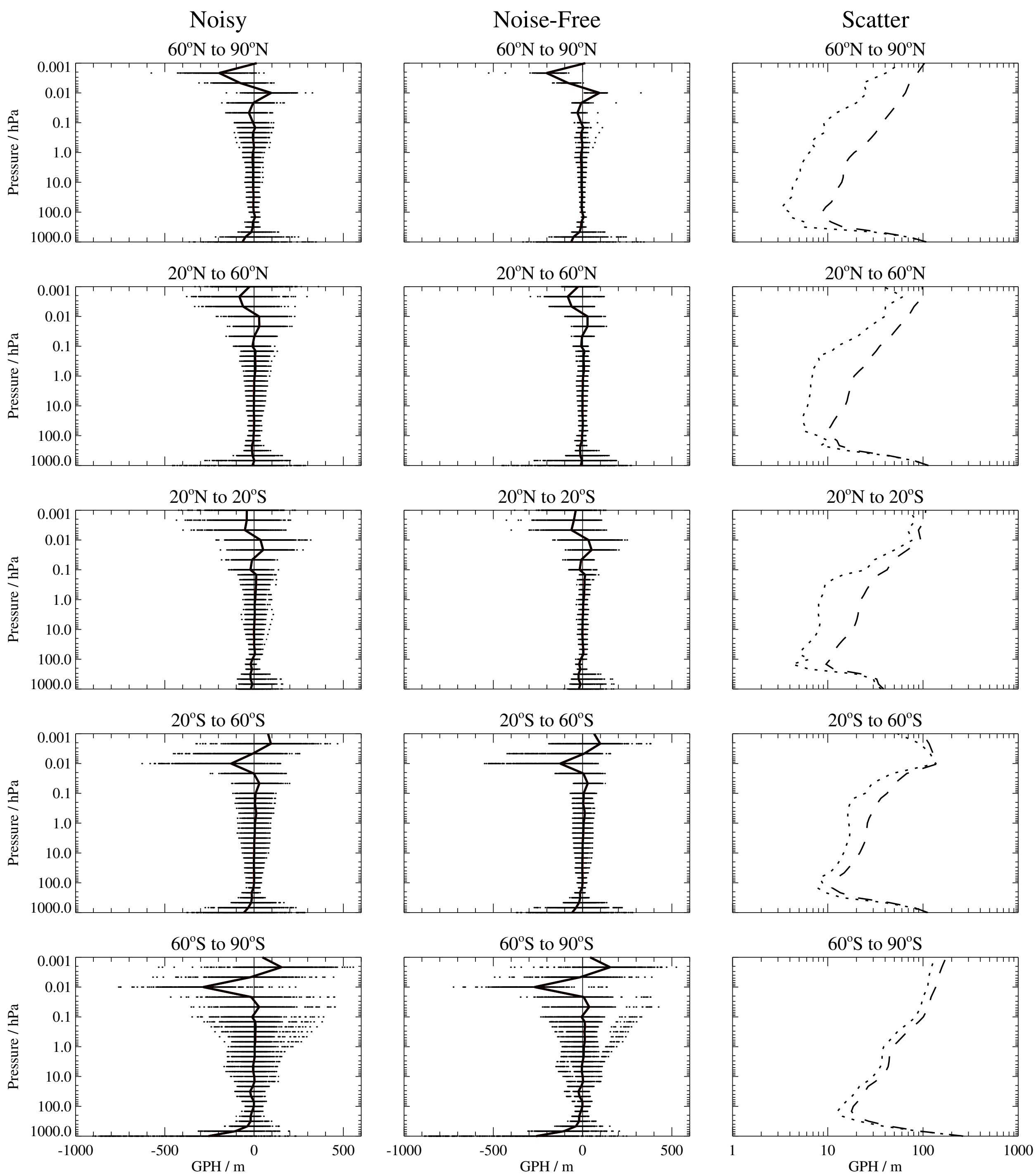


Figure 3.15: A summary of v1.5 data quality for GPH as figure 3.14 for the `2000d276` test data set.

where

$$\kappa_{z\leq 2.5} = 67.4018\,\text{m/K} \tag{3.3}$$

$$\kappa_{z>2.5} = (1 + 0.02(z - 2.5)^2)\,67.4018\,\text{m/K}, \tag{3.4}$$

σ^{ref} is the precision of `refGPH-Core`, and σ^{T} is the precision of the standard temperature profile. The GPH data should be ignored (i.e., the precision should have been set negative)

- at all levels if the `refGPH` precision used in its calculation is negative.
- at a given level if the corresponding temperature precision at that level or any level between it and the reference level is negative.

Data screening

Pressure range (316 – 0.001 hPa): Values outside this range are not recommended for scientific use.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, as they are strongly influenced by the *a priori* (see section 1.3).

Status flag: The GPH `Status` field is not correctly set. The standard temperature `Status` should be used in its place. Any profile for which `Status` is an odd number should not be used (see section 1.4).

Quality field: The GPH `Quality` field is not correctly set. The standard temperature `Quality` should be used in its place. Profiles with a value of the temperature `Quality` flag (see section 1.4) less than 1.0 should not be used.

Artifacts

- MLS 100 hPa GPH is higher than GMAO GEOS-4 by 0 – 300 m.
- The estimate (from preliminary valudation) of a 1 – 2 K warm bias in v1.5 MLS temperature in the stratosphere will lead to high biases of order 1% or less in deduced layer thicknesses.

Priorities for future data version(s)

- Fix the software to correctly write GPH precision, `Quality` and `Status` to the output files.
- Improve temperature retrieval, as GPH is integrated temperature from the 100 hPa reference level.

3.7 Water vapor

Swath name: `H2O`

Useful range: 316 – 0.1 hPa

Vertical resolution: 3 to 7 km

Contact: William Read (troposphere), **Email:** <bill@mls.jpl.nasa.gov>
Hugh Pumphrey (stratosphere/mesosphere), **Email:** <H.C.Pumphrey@ed.ac.uk>

The standard water vapor product is taken from the 190 GHz (Core+R2A) retrieval. It is unusual among MLS products in that it is assumed that log(Mixing ratio), and not mixing ratio itself, varies linearly with log pressure. For this reasons, scientific studies considering averages of MLS water vapor data should perform the averaging in log space.

Simulations

The scatter in the data is much smaller than the precision estimate. This is because the radiance errors provided to the retrieval formula are inflated to as much as 2 K. This is done to account for unexplained systematic errors which would otherwise cause poor convergence in the retrieval. The inability of the software to fit the water vapor radiances to better than 1 – 2 K is one of the reasons why the scatter in the troposphere is as poor in the noise-free case as in the noisy case.

Vertical resolution

Based on Figure 3.20 , the vertical resolution for H_2O is 2.7 – 3 km at pressures greater than 100 hPa, increases to $\sim$4 km for pressures less than 46 hPa, remaining constant throughout the stratosphere and degrades to 6 km and 7 km near 1 hPa and 0.1 hPa (the top recommended level), respectively.

Early results and validation

Stratosphere and above: The data have been compared [Froidevaux et al., 2005] to data from four occultation instruments: ACE, HALOE, POAM III and SAGE II. The comparison is qualitatively good, but the MLS data generally show a small positive bias: 5 – 10% against HALOE, 0 – 5% against ACE and 10 – 15% against SAGE II. Against POAM III the bias is negative, and about 10 – 20%. Agreement is also good against the Mk IV and FIRS-2 balloon instruments.
Upper troposphere: Comparisons of coincident profiles (8.25 minutes $\times$ 25 km) between MLS and AIRS (v4) instruments on Aura and Aqua in the EOS A-train show average biases of -25%, 3% and 12% at 316, 215 and 147 hPa respectively (negative indicates MLS is drier). The RMS scatter of the coincident profiles is large being 58%, 73% and 53% at 316, 215 and 147 hPa respectively. Given the very close coincidences, the large scatter is most likely caused by differences in the way these instruments average water vapor in their respective measurement footprints. The Aura project is conducting its own validation campaigns. A campaign conducted from Houston from 26 October to 12 November 2004 using a tunable laser hygrometer aboard a WB-57 high altitude aircraft flown under the Aura overpasses provides some in-situ comparisons. The aircraft flies mostly at an altitude in the vicinity of 100 hPa but did a number of descents down to 350 hPa. These comparisons (from 6 flights where v01.51 data are available) which are mostly biased toward the 100 hPa altitude show MLS dry by 28%, with an RMS scatter of 14%. The various *in situ* water vapor instruments show disagreements which are the subject of ongoing studies.

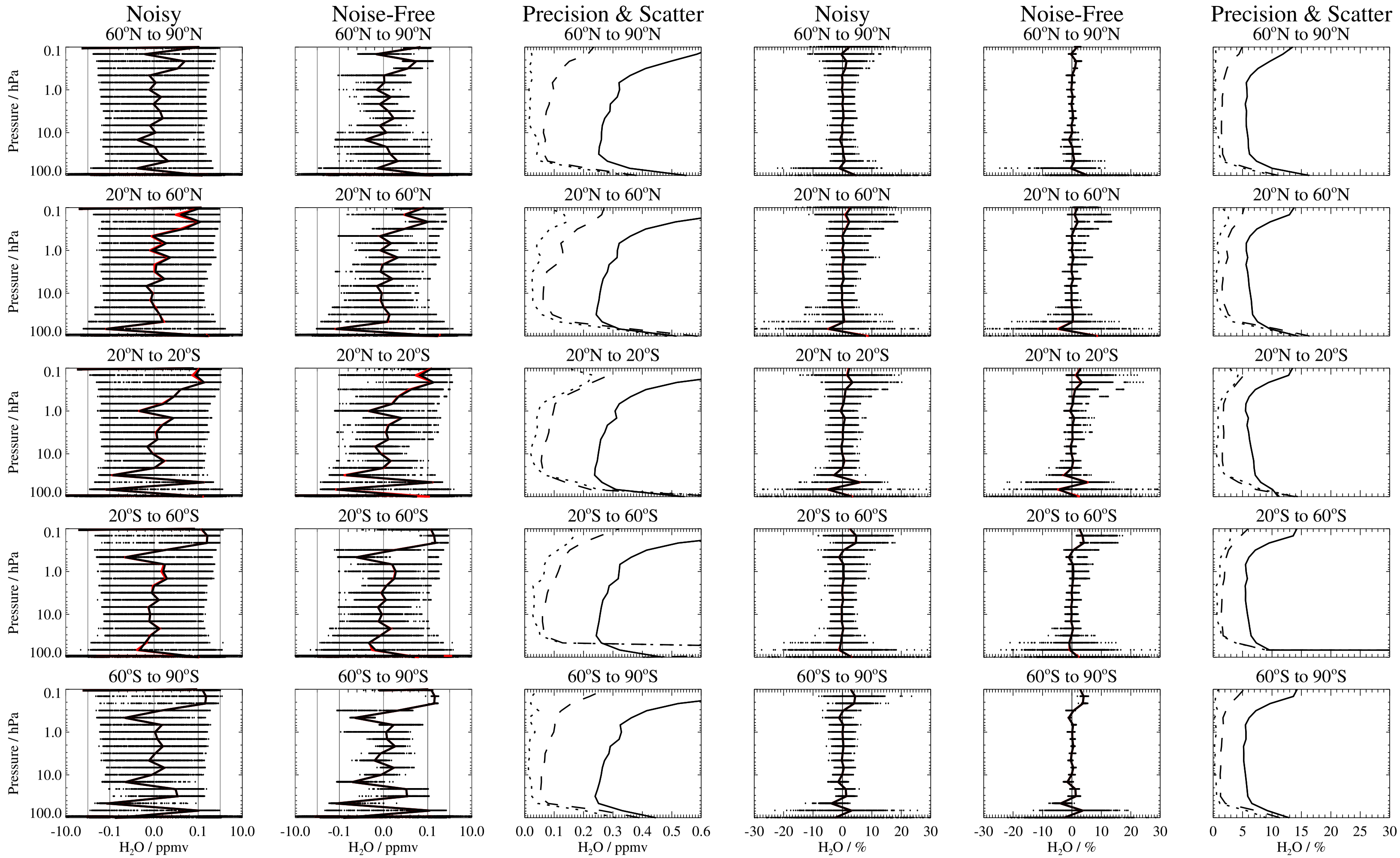


Figure 3.16: A summary of the v1.5 data quality for H_2O for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true H_2O as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of H_2O (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values. By contrast with other products, the percentage differences here are computed point by point rather than as a percentage of the mean truth. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

H_2O

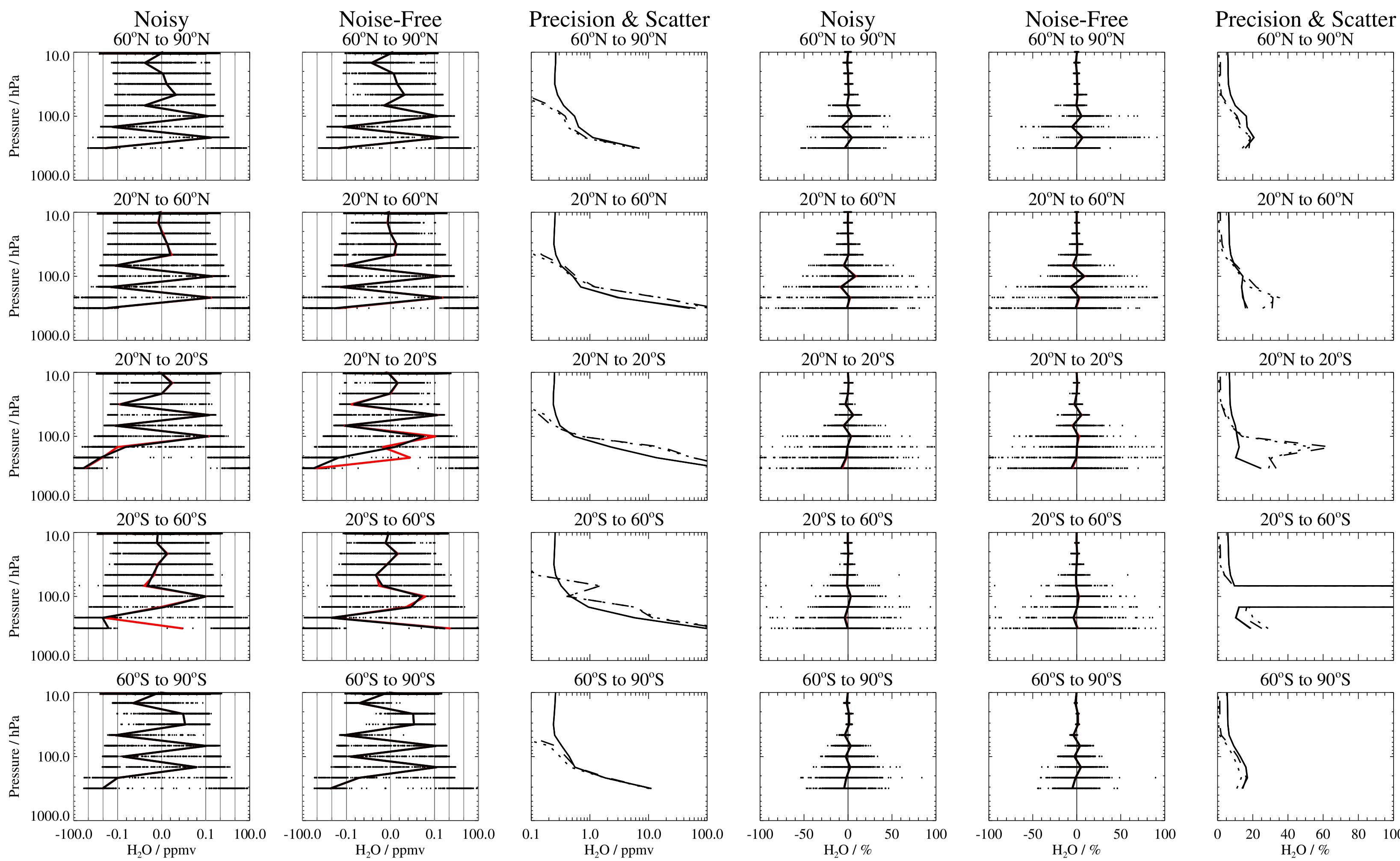


Figure 3.17: A summary of v1.5 H_2O for the `1996d051` data set as figure 3.16 with scales chosen to emphasize tropospheric amounts. By contrast with other products, the percentage differences here are computed point by point rather than as a percentage of the mean truth. This accounts for the anomalies seen at 100 hPa in the 20°S–60°S latitude bin. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

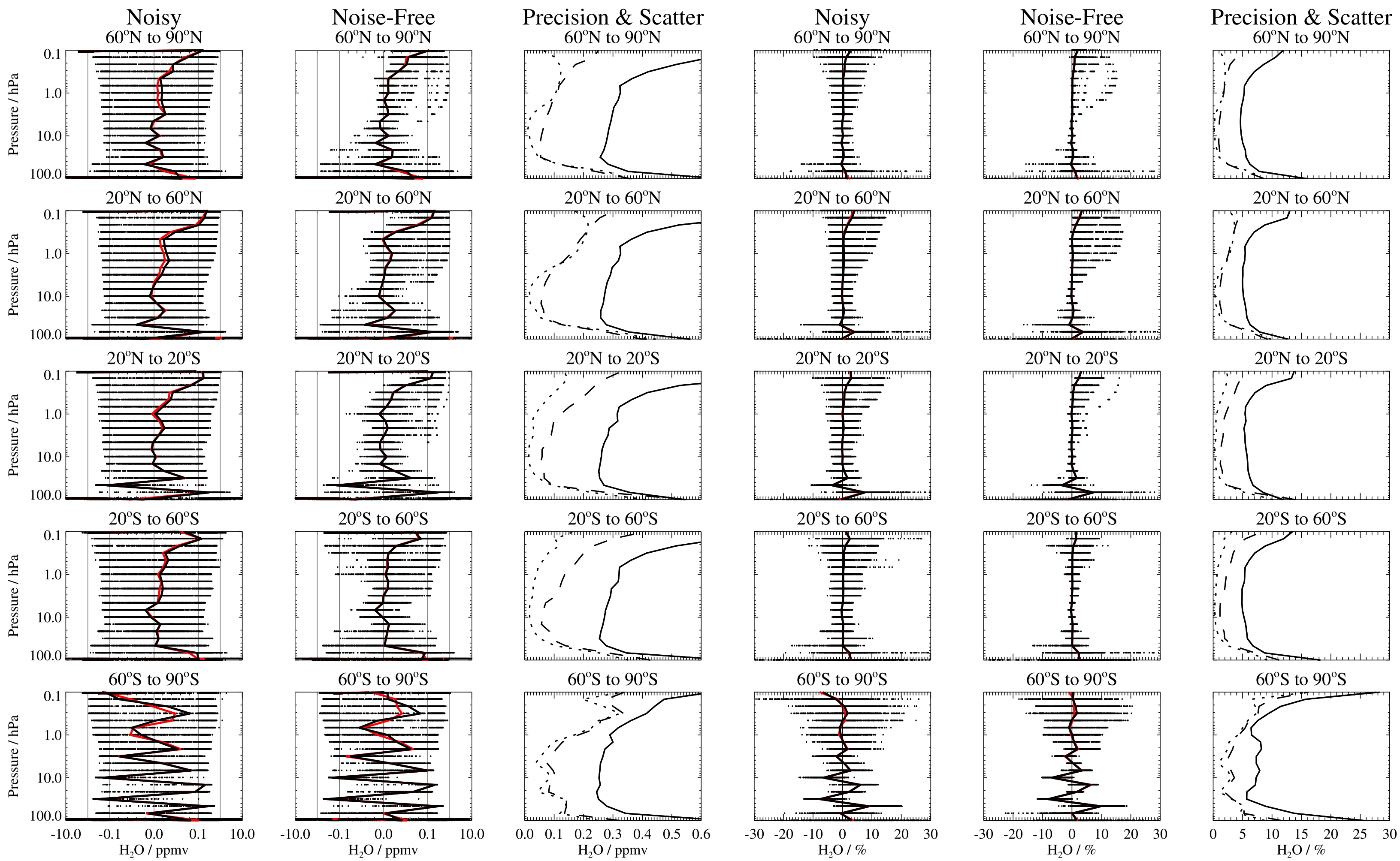


Figure 3.18: A summary of v1.5 data quality for H_2O as figure 3.16 for the `2000d276` test data set. By contrast with other products, the percentage differences here are computed point by point rather than as a percentage of the mean truth. Some of the plots in this figure use a mixed logarithmic/-linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

H_2O

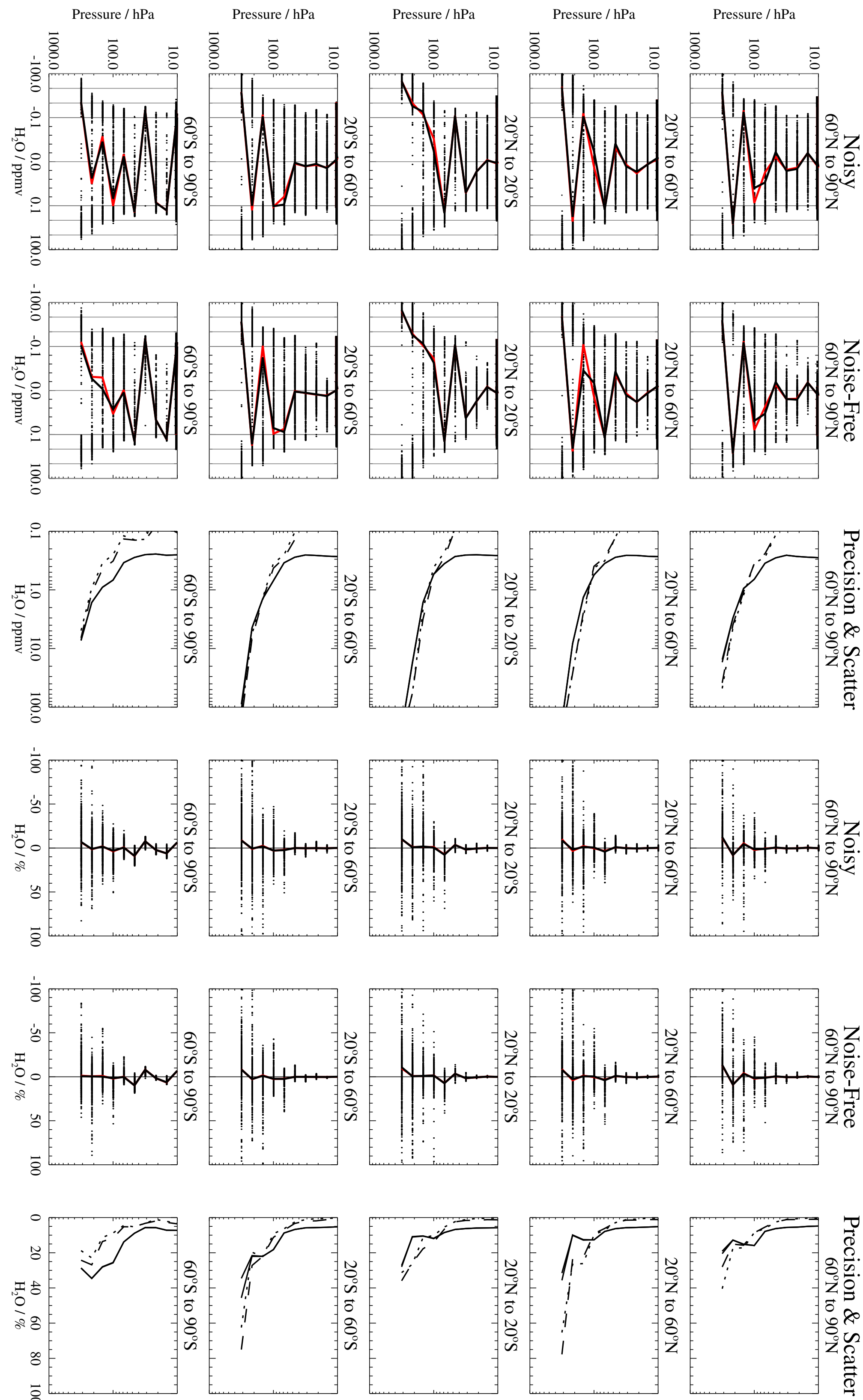


Figure 3.19: A summary of v1.5 data quality for H_2O as figure 3.17 for the `2000d276` test data set. By contrast with other products, the percentage differences here are computed point by point rather than as a percentage of the mean truth. Some of the plots in this figure use a mixed logarithmic/-linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

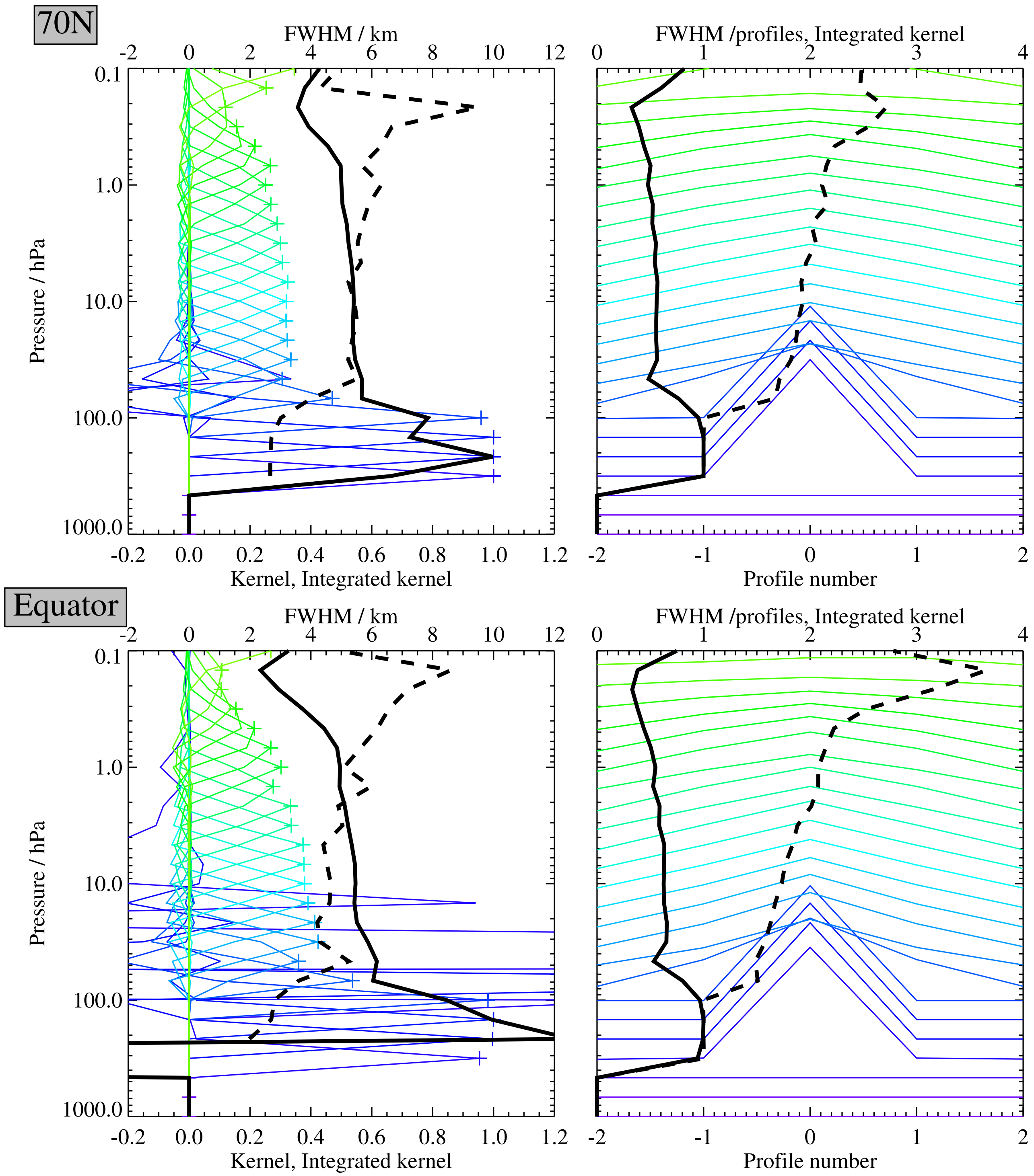


Figure 3.20: The left hand plots show the vertical averaging kernel for H_2O for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

Data screening

Pressure range (316 – 0.1 hPa): Values outside this range are not recommended for general use.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3). Users may note that values between 0.1 and 0.01 hPa, which always have negative estimated precisions, are geophysically reasonable. Data in this region should be usable in future versions, but in v1.5 they should only be used with great caution and in very close consultation with the MLS team.

Log space: Any averaging performed in scientific studies should be performed in log(vmr) space.

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: An examination of several months of v1.5 data indicates that clouds do not have a significant impact (outside the noise) on H_2O profiles down to 68 hPa. Depending on the extinction of the cloud, they can affect H_2O at 100, 147, 215 and 316 hPa. Strong cloud interference causes positive mixing ratio spikes of a few ppmv at 100 hPa along the Aura orbital track. At 215 and 316 hPa, strong cloud interference causes near zero VMR spikes. The 147 hPa level can go either way. Such effects are infrequent, affecting less than 10 profiles per day out of $\sim$3500.

Quality field: Radiance error inflation for the 190 GHz bands in v1.5 causes the `Quality` values for water vapor to be artificially large; instead of being between 0 and 1, they are typically between 0 and 25. The fit between measured and re-calculated radiances is usually worst in the upper troposphere and can often be poor there and normal in the middle atmosphere. As a result, the value of `Quality` is not a good indicator of the usefulness of the H_2O data in the stratosphere and mesosphere. Profiles with `Quality` less than 0.02 should be filtered out as a precaution but this will remove only a small number of profiles, most of which are unusable anyway on the basis of the `Status` flags.

In the troposphere (pressures $\geq$ 100 hPa), it is recommended that only profiles having `Quality` ≥ 0.3 be used. Profiles having `Quality` < 0.3 are usually the ones adversely impacted by clouds and such screening will eliminate some obviously bad profiles without rejecting an excessive amount of good data; however, there will be some poor retrievals that will not be identified. These usually manifest themselves as unusually dry values at 316 hPa with a `Quality` value less than 5. Therefore the 316-hPa H2O data should only be used where `Quality`>5.

Artifacts

Profiles often have a vertical oscillation in the lower stratosphere, with the values at odd levels (68, 33, 15 hPa) persistently higher (or lower) than at the even levels (100, 46, 22 hPa). Upper tropospheric H_2O profiles in the tropics usually in the presence of very thick clouds sometimes have mixing ratios $<$1 ppmv; this only affects $\sim$10 profiles per day.

Priorities for future data version(s)

- Eliminate vertical oscillations in lower stratosphere.
- Choose regularization (smoothing) parameters so that data are usable in upper mesosphere.
- Retrieve H_2O on 12 levels per decade pressure (double the current sampling) in the troposphere and lower stratosphere.

Other notes

The choice to retrieve log(mixing ratio) was made to provide a better match with the rapid decrease of mixing ratio with height in the troposphere. It has little bearing on the product in the stratosphere and lower mesosphere. In the upper mesosphere where the mixing ratios are small and the signal-to-noise ratio is poor, we would expect some negative values to be returned for the mixing ratio, as described in section 1.5. The choice of log(Mixing ratio) as the retrieved quantity means that the mixing ratio of water vapor is always positive.

3.8 Hydrogen chloride

Swath name: `HCl`

Useful range: 100 – 0.22 hPa

Vertical resolution: 3 to 7 km

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

The standard product for version 1.5 HCl is taken from the 640 GHz (Core+R4A) retrieval.

Simulations

Simulations (see Figures 3.21 and 3.22) indicate excellent closure for HCl, typically to better than ∼1%. Systematic biases (usually positive) tend to increase to 0.1 ppbv or more at the lowermost pressure (147 hPa); this can amount to more than 30%, for the small abundances often found at this altitude. This, and the fact that the random error also increases significantly there leads us to be cautious about HCl below 100 hPa, except possibly at high latitudes, where larger abundances can be found. The RMS scatter about the 'truth' (for noisy retrievals) is slightly (20%) lower than the estimated precision in the lower stratosphere and up to 50% lower in the lower mesosphere. Clouds tend to cause some (mostly positive) biases, but mainly at 147 hPa, where the estimated precision is also increasing, so the effect on real data will not be obvious. Some profiles incur vertical oscillations at high latitudes, although this is usually within the estimated noise of the measurements.

Vertical resolution

Based on Figure 3.23, the vertical resolution for HCl is ∼3 km in the lower stratosphere, and degrades to 5 – 6 km near 1 hPa and 7 km at the top recommended level of 0.2 hPa.

Early results and validation

The estimated single-profile precision ranges from ∼0.1 ppbv (lower stratosphere) to 0.5 ppbv (lower mesosphere), or 5 to 15 %. This is typically close to the scatter based on the retrieved profile variability, evaluated in a narrow latitude band centered around the equator, where atmospheric variability is expected to be small, except at the top end of the profile, where the scatter tends to be somewhat smaller than the estimated precision; this indicates an increasing influence from the *a priori*, although not to an extent that affects the retrieved abundances much. Comparisons of MLS and HALOE HCl for January-March, 2005 [Froidevaux et al., 2005] indicate that MLS HCl abundances are typically high, relative to HALOE, by ∼0.2 to 0.4 ppbv (∼10 to 15%). In contrast, MLS HCl is typically within ∼5 % of the ACE HCl values, certainly in the upper stratosphere and in the more quiescent SH lower stratosphere. Larger differences are observed in the more disturbed conditions of NH high latitude winter. Similar patterns are observed between HALOE, MLS, and ACE zonal means in August and September at low and high latitudes. The exact cause of the disagreement with HALOE is not known at this time, but there have been indications that HALOE HCl data were on the 'low side' of other observations (from satellite, balloons, aircraft) by ∼10 – 15%. Comparisons of MLS HCl versus balloon-borne measurements in September 2004 from Ft. Sumner, New Mexico, indicate good agreement, generally within the combined random errors. Despite the bias issue versus HALOE, we find that the HCl latitudinal variations agree well between HALOE and MLS.

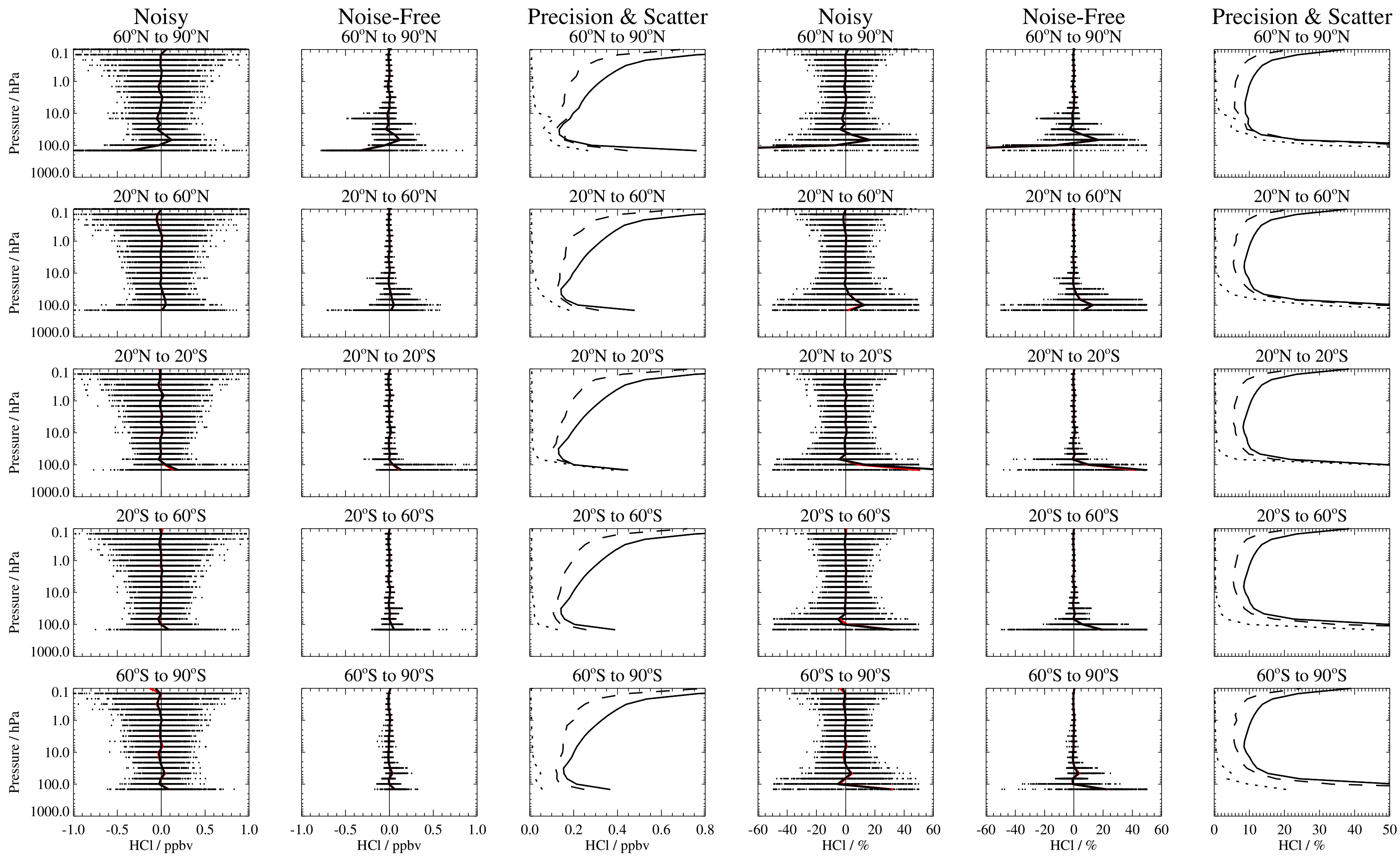


Figure 3.21: A summary of the v1.5 data quality for HCl for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true HCl as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of HCl (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values.

HCl

HCl

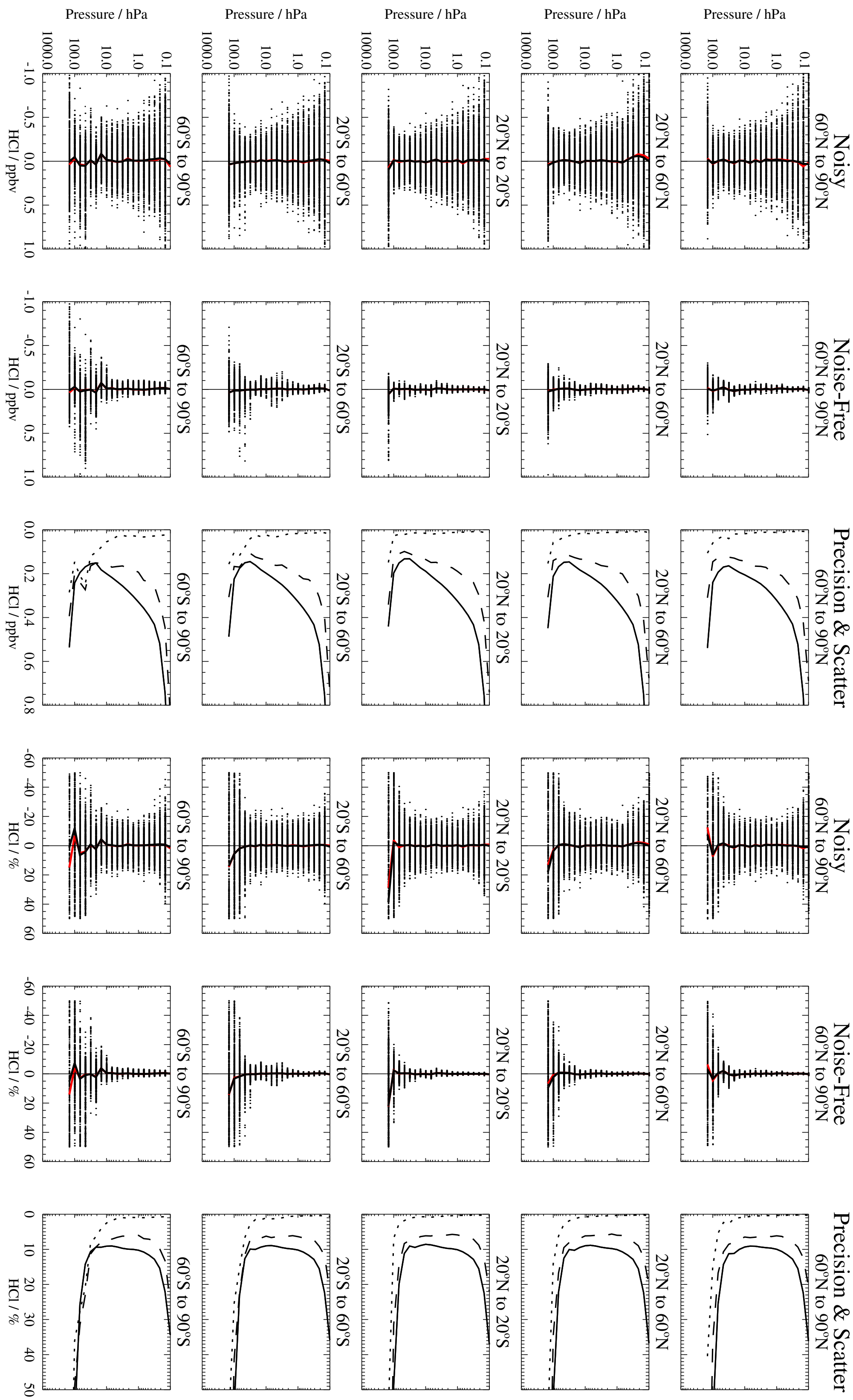


Figure 3.22: A summary of v1.5 data quality for HCl as figure 3.21 for the 2000d276 test data set.

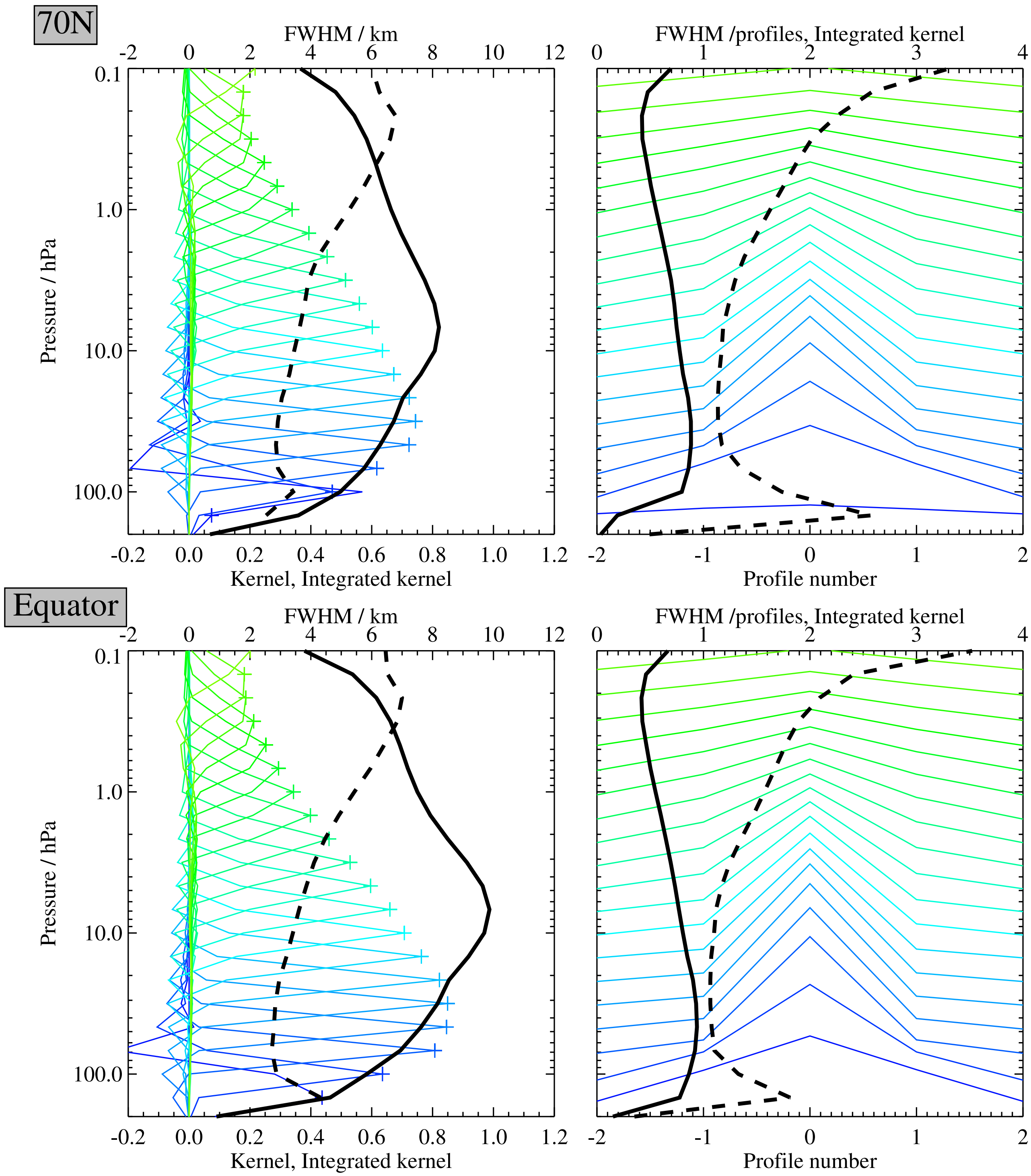


Figure 3.23: The left hand plots show the vertical averaging kernel for HCl for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

Data screening

Pressure range (100 – 0.22 hPa): Values outside this range are not recommended for scientific use.The 0.22 hPa limit is conservatively based on single-profile precisions and a desire for limited influence from the *a priori*; these is useful radiance information at higher altitudes. In the upper stratosphere and lower mesosphere, HCl can be used as an indicator of total chlorine; some averaging (of 50 to 100 profiles) is required to reduce the noise to less than a few percent.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: An examination of several months of v1.5 data indicates that clouds do not have a significant impact (outside the noise) on HCl profiles down to 147 hPa; there is currently no apparent need to discard profiles or profile portions where `Status` values indicate the existence/influence of clouds (see section 1.4).

Quality field: Profiles with a value of the `Quality` field (see section 1.4) less than 1.5 should not be used. This flag will throw out a few outliers (with very high or low abundances), but is mostly an indication of poor radiance fits, even for reasonable-looking profiles; a very small fraction of HCl profiles (much less than 1%) will be discarded via this screening.

HCl

Artifacts

Some negative average values of order −0.1 to −0.3 ppbv are sometimes observed below 10 hPa when very low values are present in the winter SH polar vortex. Small negative biases are also apparent more frequently at 147 hPa (not a recommended level for use) in both NH and SH winter polar vortex regions.

Priorities for future data version(s)

- Understand and remove the small negative biases that are sometimes evident for very low HCl polar winter conditions (see artifacts above).
- Attempt to improve the retrievals at the lowest altitudes.

HCl

3.9 Hydrogen cyanide

Swath name: `HCN`

Useful range: 10 – 1.4 hPa

Vertical resolution: 6 km

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

HCN is produced by the 190 GHz (Core+R2B) retrieval.

Simulations

The signal from the HCN molecule is not strong and as a result the HCN product is noisy and will require some form of averaging for most purposes. The spectral line of HCN lies in the lower sideband of the radiometer, at 177 GHz. This spectral region is relatively free of interfering lines but the double sideband nature of the measurement mixes the HCN signal with much stronger signals from O_3 and HNO_3 in the upper sideband. This interference makes the retrieval of HCN problematic in the lower stratosphere. Figures 3.24 and 3.25 give some indication of the problem but inspection of HCN retrieved from the measured radiances suggests that it is worse than in the simulations.

HCN

Vertical resolution

Based on Figure 3.26 , the vertical resolution for H_2O is 6 km between 10 hPa and 1 hPa.

Early results and validation

Comparisons against historic measurements suggest that the retrieved data are reasonable in the upper stratosphere (10 hPa – 1 hPa). In the lower stratosphere (100 hPa – 14 hPa) they are quite clearly wrong and should not be used.

Data screening

Pressure range (10 hPa – 1.4 hPa): Values outside this range are not recommended for scientific use.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: As v1.5 HCN can only be received at altitudes well above the troposphere the cloud flags in `Status` may be ignored.

Quality field: The normal value for `Quality` for HCN is close to 2. Profiles with `Quality` less than 1.0 should be rejected.

Artifacts

None noted in the recommended pressure range.

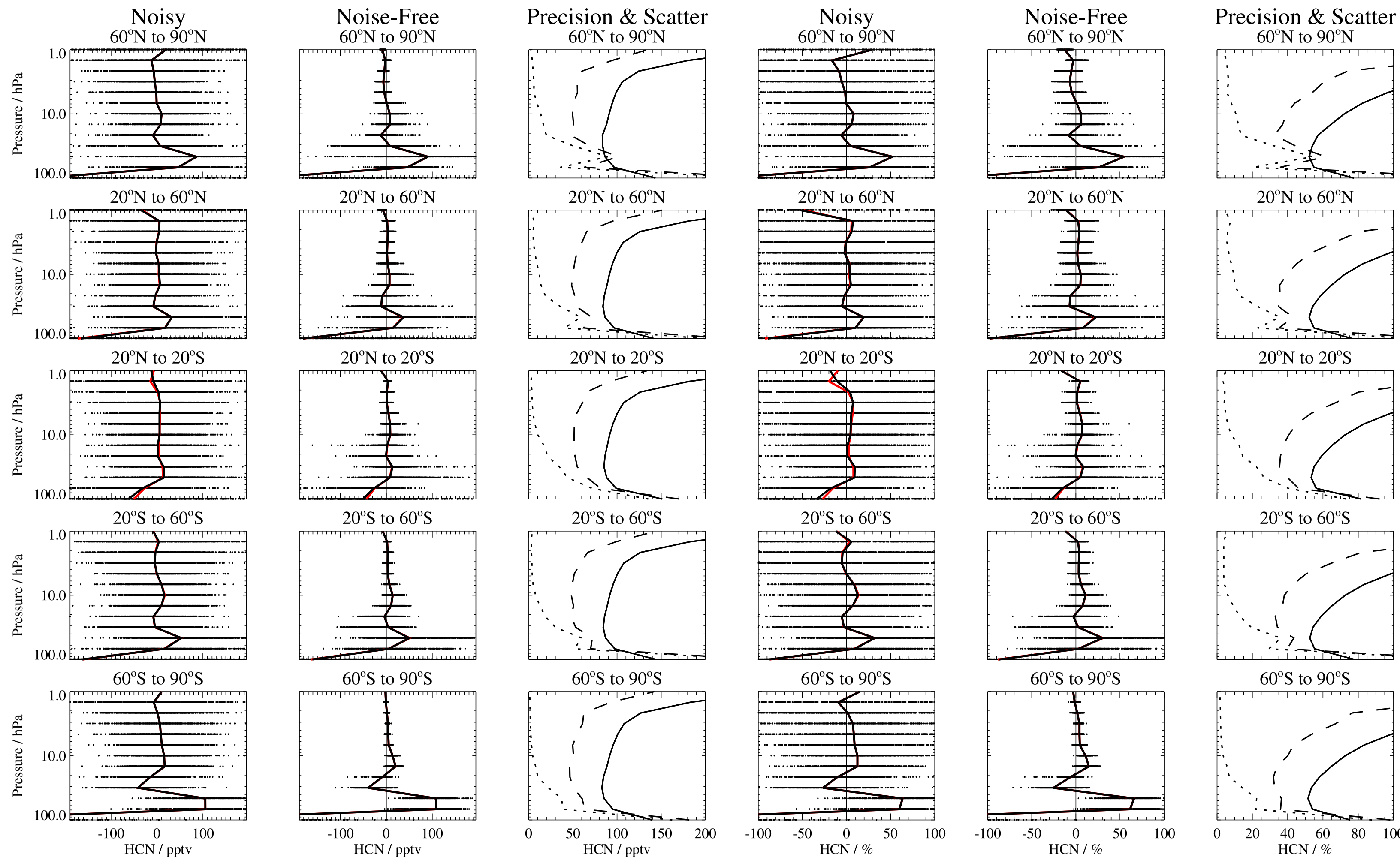
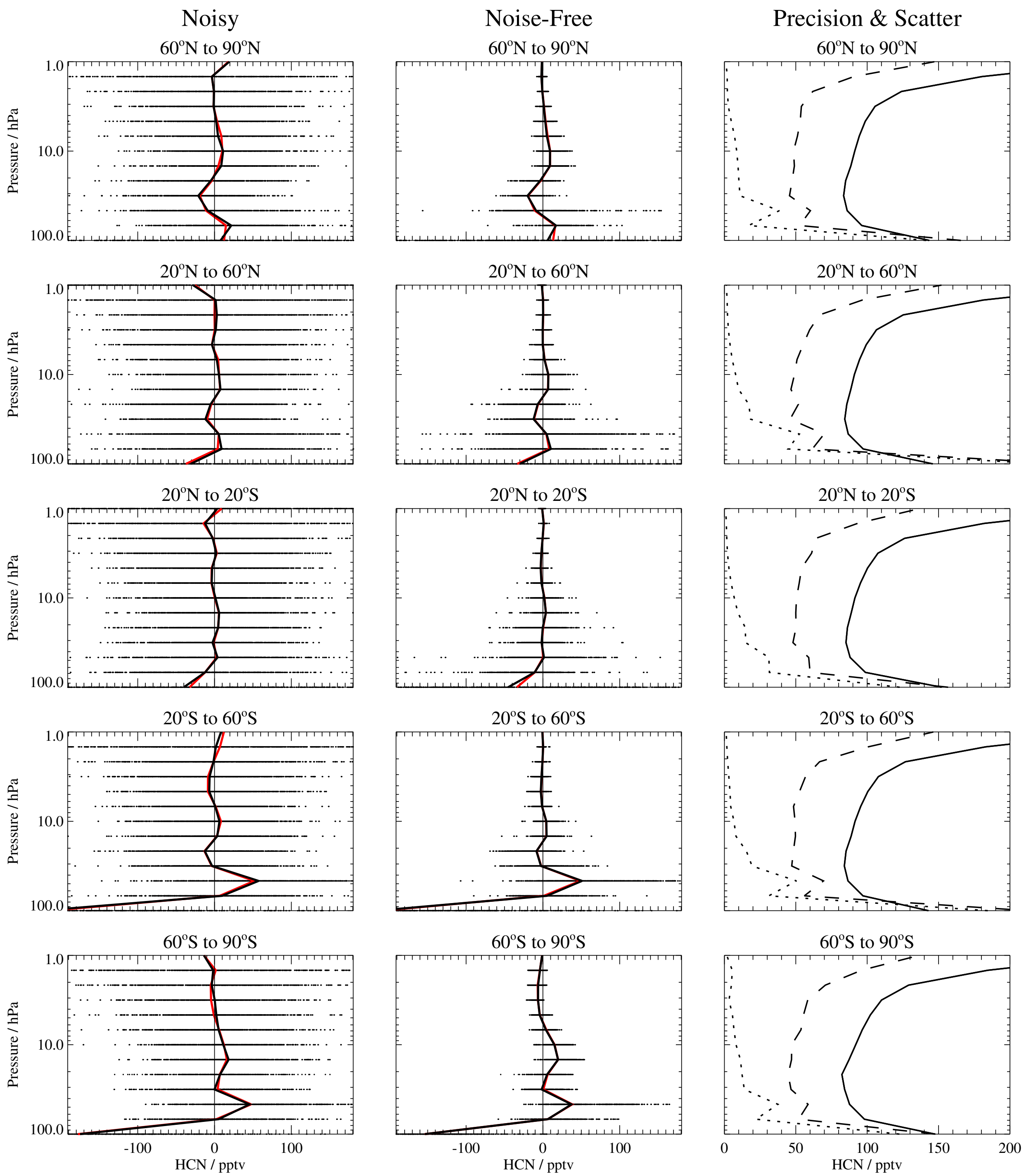


Figure 3.24: A summary of the v1.5 data quality for HCN for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true HCN as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of HCN (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values.

HCN



HCN

Figure 3.25: A summary of v1.5 data quality for HCN similar to figure 3.24 except for the `2000d276` test data set. The percentage plots are omitted here as the 'true' values are zero.

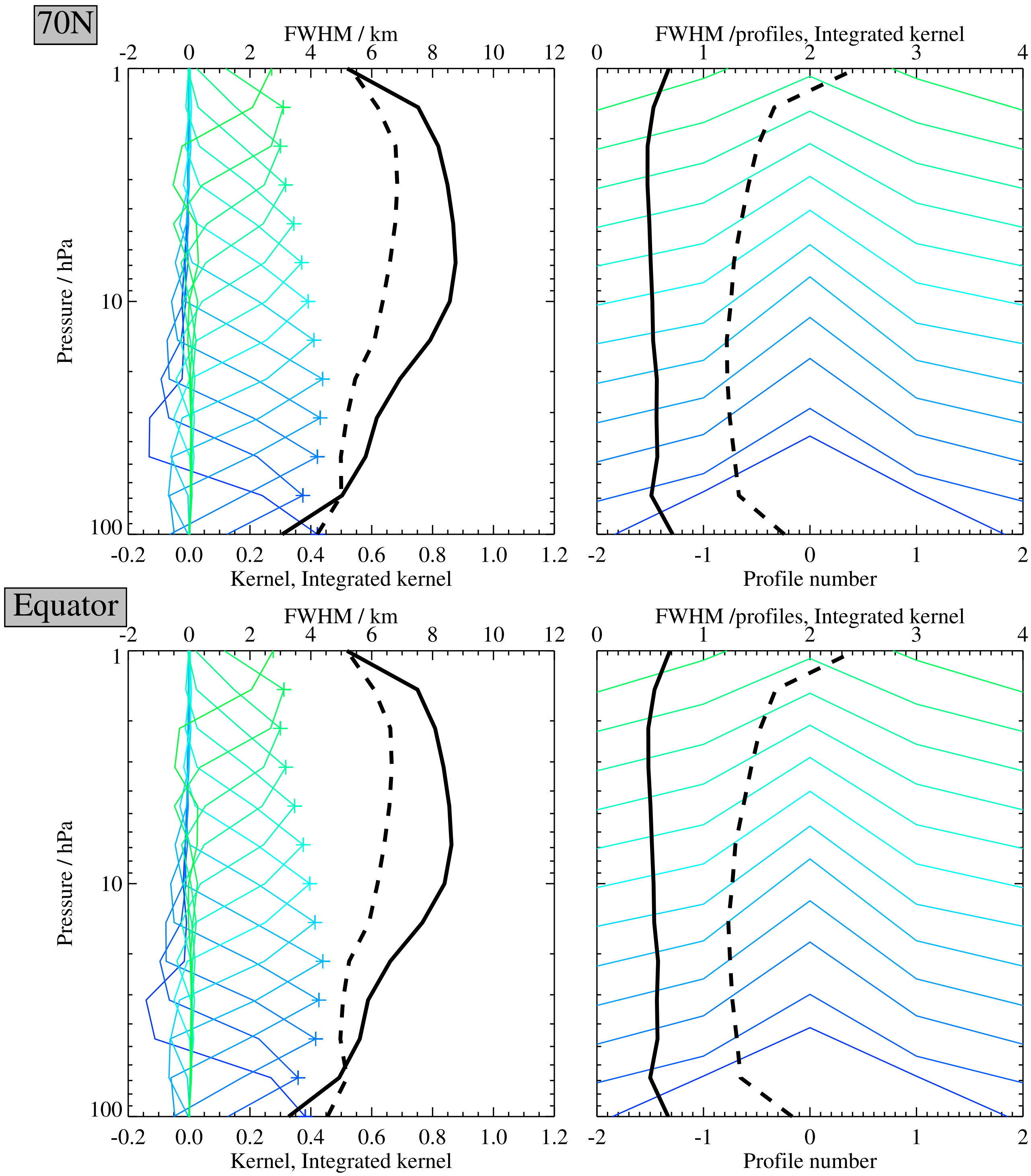


Figure 3.26: The left hand plots show the vertical averaging kernel for HCN for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

3.10 Nitric acid

Swath name: `HNO3`

Useful range: 147 – 3.2 hPa

Vertical resolution: 3.5 to 4.5 km

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

The standard product for version 1.5 HNO_3 is taken from the 240 GHz (Core+R3) retrieval at and below 10 hPa, and from the 190 GHz (Core+R2B) retrieval at and above 6.8 hPa.

Simulations

Simulations (see Figures 3.27 and 3.28) indicate that average biases are small ($<$0.3 ppbv) at most latitudes over the range 147–3.2 hPa, with an overall accuracy of better than 10%. However, the simulations suggest that large systematic biases limit the scientific usefulness of the v1.5 HNO_3 retrievals outside of this range.

Vertical Resolution

Based on Figure 3.29, the vertical resolution of the standard HNO_3 product is estimated to be ~3.5 km over the range 147 to 10 hPa, degrading to ~4.5 km at 3.2 hPa.

Early Results and Validation

Over most of the recommended vertical range, the estimated single-profile precision reported by the Level 2 software varies from ~1.0 to 1.5 ppbv; the observed scatter in the data, evaluated in a 20°-wide latitude band centered around the equator where atmospheric variability is expected to be small, suggests a measurement precision of ~1 ppbv throughout the profile. Preliminary comparisons with a climatology based on seven years of UARS MLS HNO_3 measurements [Santee et al., 2004] suggest that EOS MLS HNO_3 may be biased high by several ppbv near the profile peak. Much closer agreement with the UARS climatology is generally found at other latitudes/altitudes/seasons. Comparisons of HNO_3 profiles from MLS and ACE at middle and high latitudes in both hemispheres over the January to March 2005 time period [Froidevaux et al., 2005] indicate that, in an average sense, MLS HNO_3 is high relative to ACE by at least 2 – 3 ppbv (~30%) at the levels surrounding the profile peak. Average agreement between the two satellite measurements is better (typically within ~10%) near the top and bottom of the profile. Despite the apparent offset between MLS and ACE near the profile peak, however, comparisons of nearly-coincident individual measurements show good agreement in capturing the overall shapes of the HNO_3 profiles and tracking variations in them. Comparisons with HNO_3 measurements from the FIRS-2 and Mark-IV instruments obtained during a balloon campaign from Ft. Sumner, NM in September 2004 lead to similar conclusions: MLS mixing ratios exceed those measured by the balloon instruments by as much as 3 ppbv at the levels around the profile peak, with agreement typically much better at the top and bottom of the vertical range [Froidevaux et al., 2005]. The discrepancies between HNO_3 abundances measured by MLS and those measured by ACE, FIRS-2, and Mark-IV may arise in part because of uncertainties in either the infrared or the microwave spectroscopy; this possibility is under investigation. The altitude, latitude, and seasonal dependence of the apparent high bias in the MLS version 1.5 HNO_3 data will be explored in more detail in future validation studies, both through analysis of potential shortcomings in the MLS retrieval system and comparisons with additional correlative (ground-based, aircraft, balloon, and satellite) data sources.

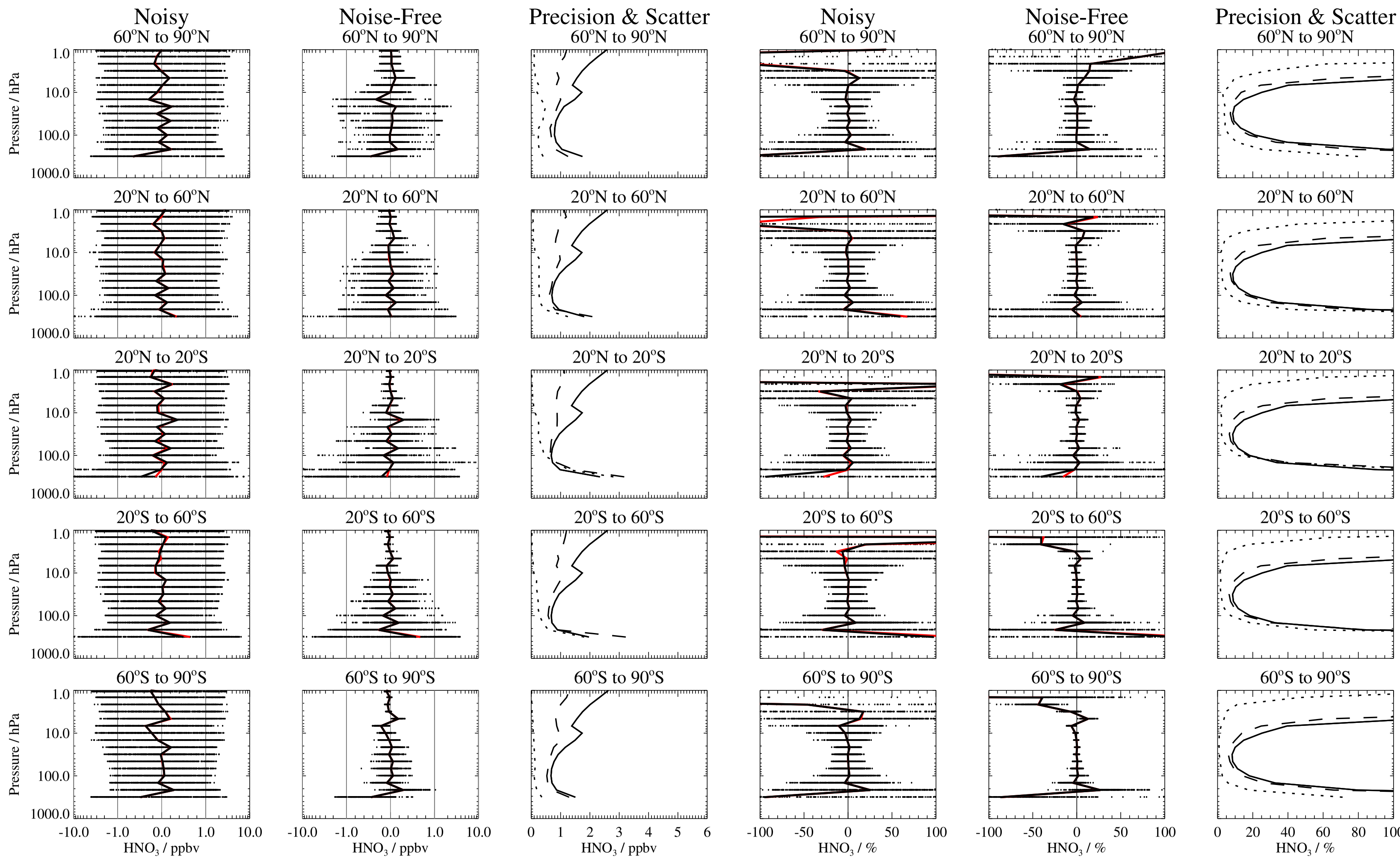


Figure 3.27: A summary of the v1.5 data quality for HNO_3 for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true HNO_3 as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of HNO_3 (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values.

HNO_3

HNO$_3$

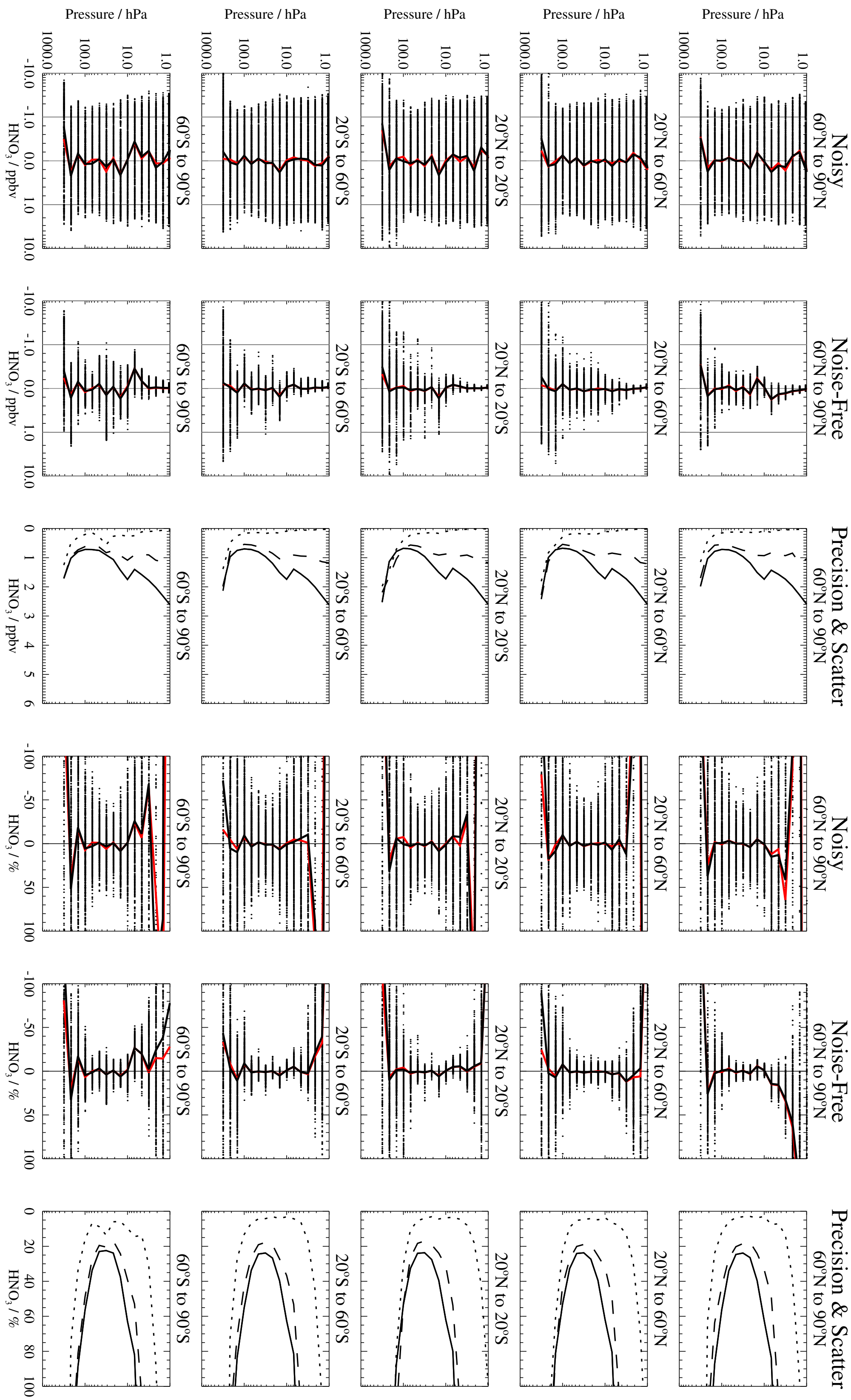


Figure 3.28: A summary of v1.5 data quality for HNO$_3$ as figure 3.27 for the 2000d276 test data set.

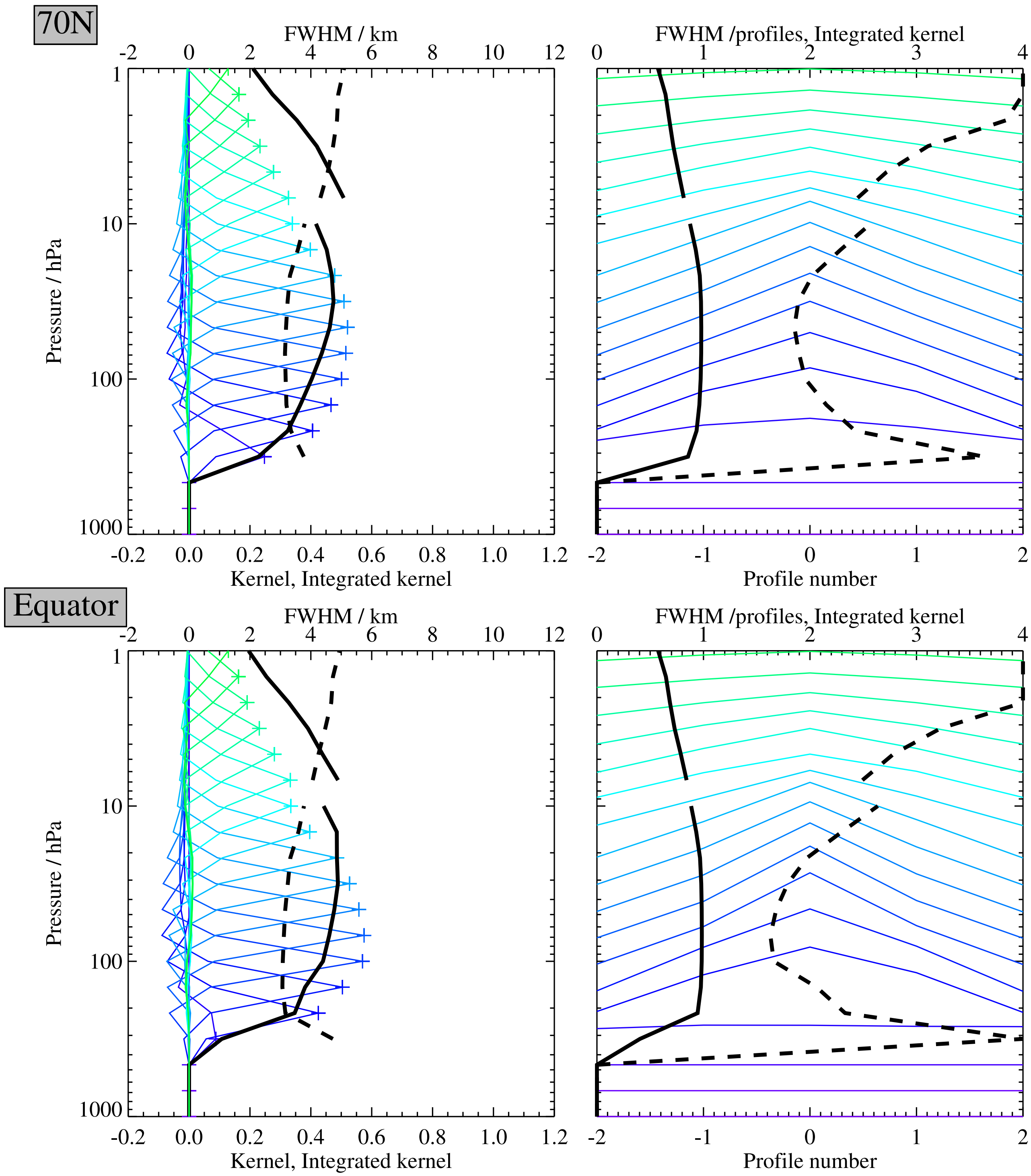


Figure 3.29: The left hand plots show the vertical averaging kernel for HNO_3 for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

Data Screening

Pressure range (147 – 3.2 hPa): Values outside this range are currently not recommended for scientific use. Averages may prove useful at 215 hPa, but determining their reliability will require further analyses.

Estimated precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: An examination of several months of v1.5 data indicates that clouds do not have a significant impact (outside the noise) on HNO_3 profiles down to 147 hPa; there is currently no apparent need to discard profiles or profile portions where `Status` values indicate the existence/influence of clouds (see section 1.4).

Quality: Virtually all HNO_3 profiles have `Quality` values (see section 1.4) well below 1.0, indicating that in general the radiance fits are not as good for this product as for many other MLS retrievals. Imposing a threshold value of 0.17 for HNO_3 `Quality` (below which a profile is discarded) throws out about 1% of data, eliminating profiles with obvious `Quality` outliers while minimizing rejection of profiles with apparently decent fits.

Artifacts

High bias: Based on comparisons with nearly-coincident satellite and balloon measurements, the MLS HNO_3 retrievals appear to be biased high by about 3 ppbv (∼30%) near the profile peak; the extent to which this is an artifact is under investigation.

Oscillations: The HNO_3 profile is often slightly oscillatory.

Priorities for future data version(s)

- Understand and mitigate (if the problem is determined to lie with the MLS retrieval system) the apparent large positive bias in HNO_3 abundances at the levels surrounding the profile peak.
- Reduce oscillations in the HNO_3 profile.
- Attempt to improve the retrievals at 215 hPa.

3.11 The peroxy radical

Swath name: `HO2`

Useful range: 22 – 0.22 hPa

Contact: Herbert Pickett, **Email:** <hmp@mls.jpl.nasa.gov>

The standard product for version 1.5 HO_2 is taken from the 640 GHz (Core+R4A) retrieval.

Simulations

Simulations (see Figures 3.30 and 3.31) indicate closure for HO_2 day/night differences to better than 10 % above 22 hPa. Without taking day/night (ascending/descending) differences the closure in the simulations is at times larger than the expected daytime HO_2 concentration. The scatter shown in the right column in these figures for the noise-free simulations at all latitudes is significantly smaller than the precision. The scatter in the noisy simulations is comparable to the estimated precision.

Vertical resolution

Based on Figure 3.32, the vertical resolution for HO_2 is 3 – 4 km in the 22 hPa to 0.22 hPa range.

Early results and validation

Significant averaging (e.g., weekly zonal means) is required to obtain useful HO_2 data from MLS observations. Averages of nighttime observations (from the descending part of the orbit), when HO_2 abundances are expected to be essentially zero show significant non zero values, indicative of biases. These need to be removed before any scientific study by taking day/night (or ascending/descending) differences. We believe that these differences will be reliable at levels at and above the 22 hPa pressure surfaces. At pressures greater than 22 hPa the bias is larger than we can confidently expect simple day/night differences to remove.

HO_2 is being validated using the balloon-borne FIRS-2 instrument. Preliminary results for September 23, 2004, for the region of Ft. Sumner, NM show excellent agreement between FIRS-2 and MLS [Pickett et al., 2005].

Data screening

Pressure range (22 – 0.22 hPa): Values outside this range are not recommended for scientific use.The 22 hPa limit is conservatively based on the size of retrieved night values of HO_2. Averages may be useful at higher altitudes than 0.22 hPa, but this will require further analysis.

Diurnal differences: Day/night differences should be taken for any scientific study.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: Within the recommended pressure range, clouds should not have any effect on HO_2 concentration. There is currently no need to discard profiles or profile portions where `Status` values indicate the existence/influence of clouds (see section 1.4).

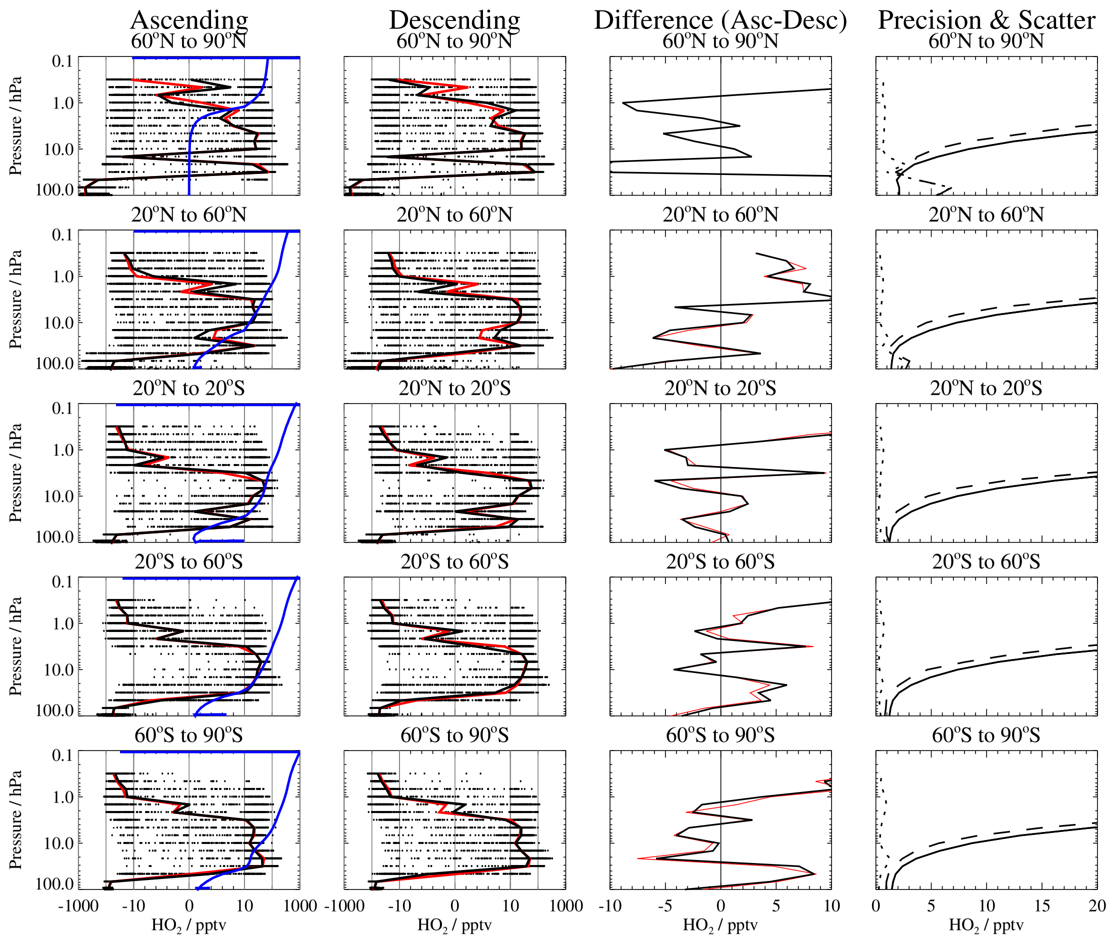


Figure 3.30: A summary of the v1.5 data quality for HO_2 for the `1996d051` test dataset. Each row of panels represents a broad latitude bin. The first two columns show, for the noise-free case, the differences between the retrieved and true HO_2 as a function of pressure for the ascending and descending phases of the Aura orbit (corresponding to mainly day and mainly night observations respectively). Also shown is a solid line that indicates the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the difference in the median biases (solid black lines in previous columns) between the ascending and descending side. The fourth column shows the mean estimated precision of monthly zonal means of HO_2 in 5° wide latitude bins (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases, scaled to correspond to the ‘scatter’ that would be expected in the monthly zonal means. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.The blue line in the first column of plots indicates a typical abundance of HO_2 for reference.

HO_2

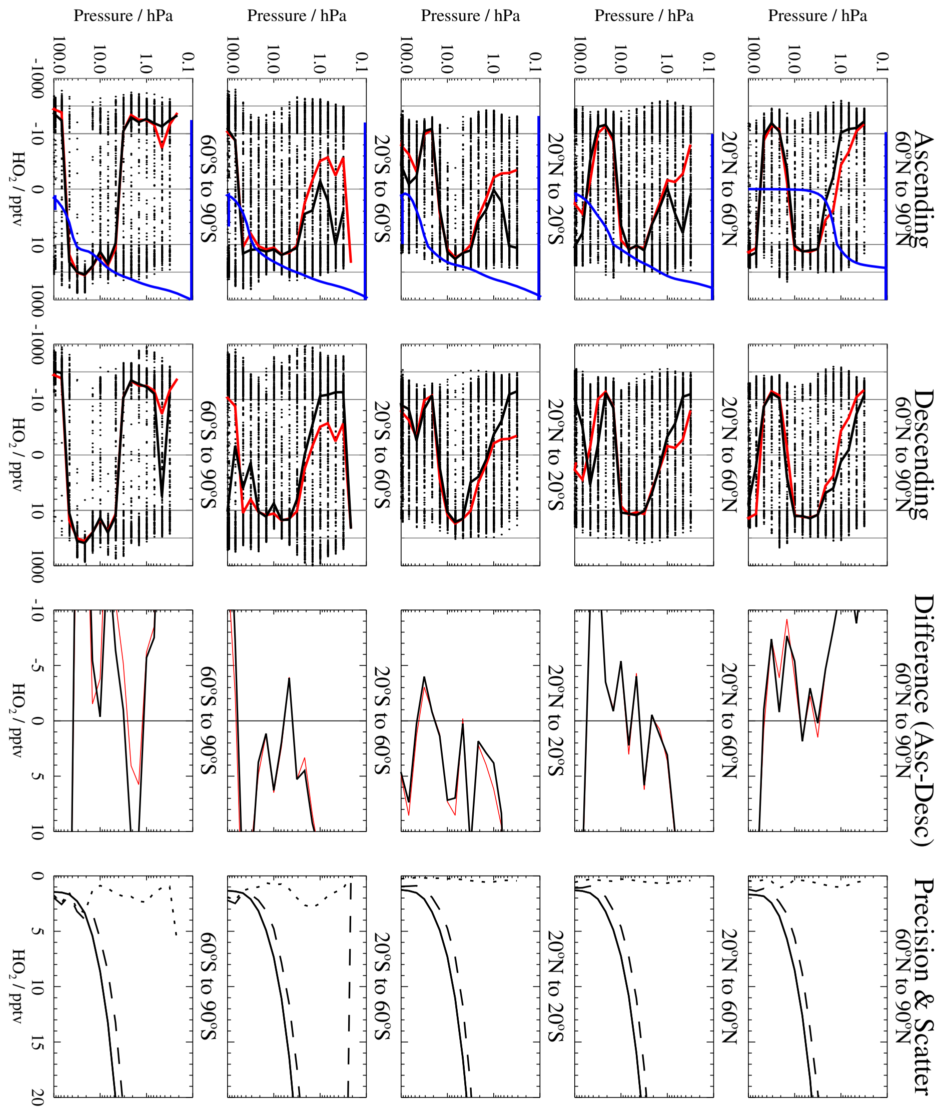


Figure 3.31: A summary of v1.5 data quality for HO_2 as figure 3.30 for the 2000d276 test data set.

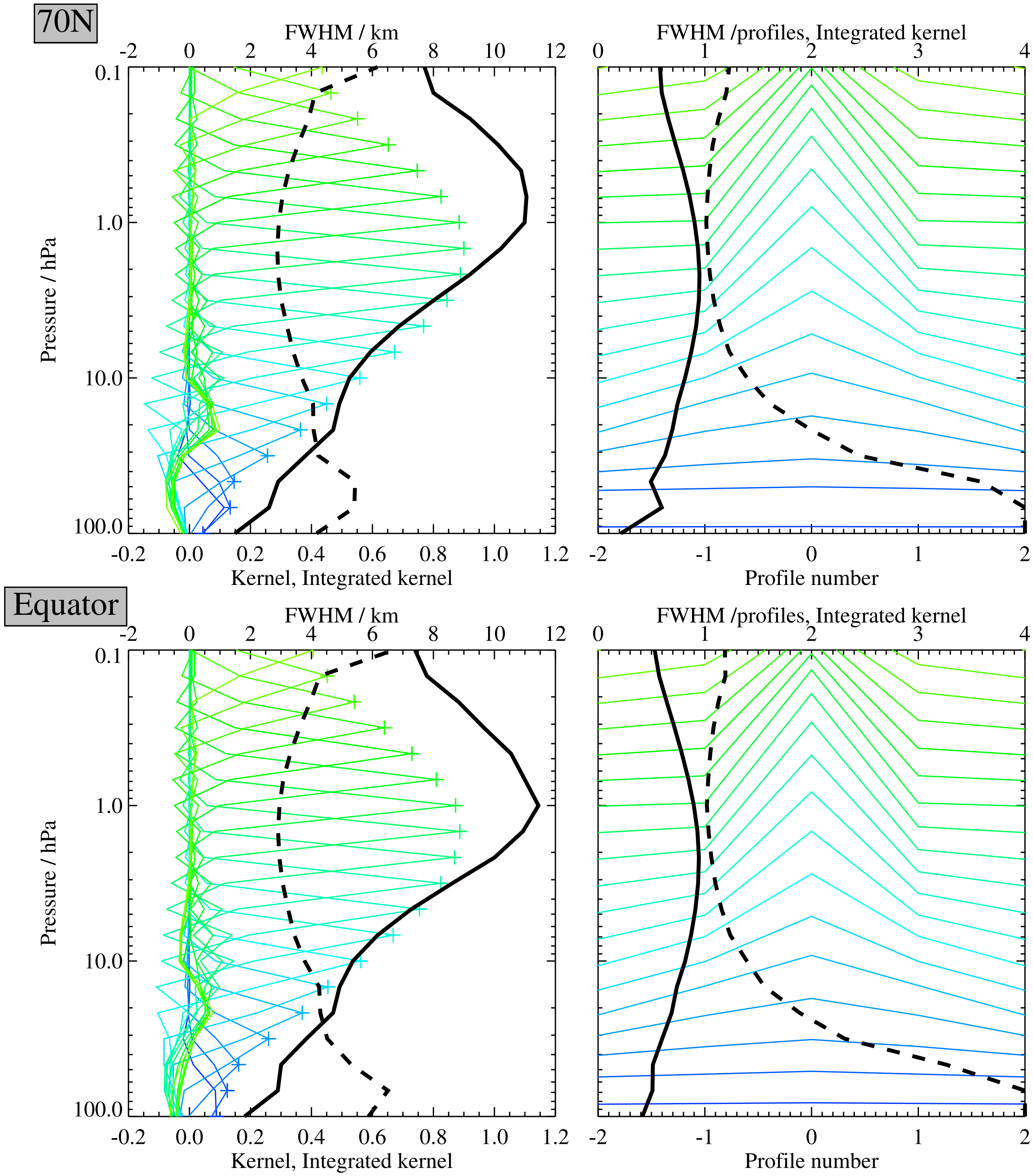


Figure 3.32: The left hand plots show the vertical averaging kernel for HO_2 for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

Quality field: Profiles with a value of the `Quality` field (see section 1.4) less than 2.5 should not be used. This flag is mostly an indication of poor radiance fits, even for reasonable-looking profiles; a very small fraction of HO_2 profiles (much less than 1%) will be discarded via this screening.

Artifacts

Use of day/night differences is recommended because of significant systematic errors in the day-only and night-only retrievals. Below 22 hPa the systematic errors are so large that the day/night difference becomes suspect.

Priorities for future data version(s)

Attempt to improve the retrievals at the lowest altitudes.

3.12 Hypochlorous acid

Swath name: `HOCl`

Useful range: 22 – 2.2 hPa.

Vertical resolution: 4 – 5 km.

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

The standard product for version 1.5 HOCl is taken from the 640 GHz (Core+R4A) retrievals.

Simulations

Simulations (see Figures 3.33 and 3.34) indicate that the weak HOCl signals will lead to v1.5 retrievals that are accurate to no better than 20%, and that small abundances at pressures larger than 46 hPa will be difficult to obtain. Simulations indicate that enhanced lower stratospheric values of 0.5 to 1 ppbv may be tracked at the 20% level, in single profiles. Real data systematics for v1.5 HOCl, however, lead us to recommend a maximum pressure of 22 hPa. Systematic biases are usually positive in the simulations, and of order 20 – 40 pptv for the mid-to upper stratosphere. The estimated precision, for monthly zonal means in 5°-wide latitude bins is under 10 pptv, or of order 10%. The rms scatter in this region (for noisy retrievals) is ∼50% lower than this estimated precision. Simulations do not indicate a significant impact from clouds for the mid-stratosphere and above. Given the noisy retrievals and the fact that the MLS HOCl product is not believed to be useful in the lowermost stratosphere, we do not need to consider in more detail the effects of clouds on the v1.5 HOCl retrievals.

Vertical resolution

Based on Figure 3.23, the vertical resolution for HOCl is ∼5 km.

Early results and validation

HOCl is a noisy product and its typical stratospheric abundance is expected to be less than ∼200 pptv, except under heterogeneously-enhanced conditions in the lower stratospheric winter polar vortex, where larger abundances of order 0.5 – 1 ppbv may occasionally be found.

We feel that zonal mean information (e.g., in 10°-wide bins) from one day's worth of MLS data is marginally useful, although monthly or bi-weekly averages will reduce the noise to more practical levels. Some HOCl enhancements are evident in the lower stratospheric high latitudes during winter. We have also performed some comparisons versus HOCl results from the SLIMCAT model; these and related analyses are currently under investigation.

Few results will exist on actual validation for HOCl, given the paucity of such data and the lack of single-profile sensitivity for MLS. Some balloon-borne profiles exist, and comparisons of MLS zonal means to these over the recommended vertical range (22 – 2.2 hPa) look encouraging. If and when other satellite retrievals of this product become available, we would want to compare to these as well.

Data screening

Pressure range (22 – 2.2 hPa): Values outside this range are not recommended for use. Very low values are obtained below 30 hPa, presumably as a result of contamination and/or poorly modeled small signals from this molecule in the lower stratosphere. There are also indications of negative averaged HOCl values in the uppermost stratosphere, which is why we limit the current upper range of usefulness to 2.2 hPa.

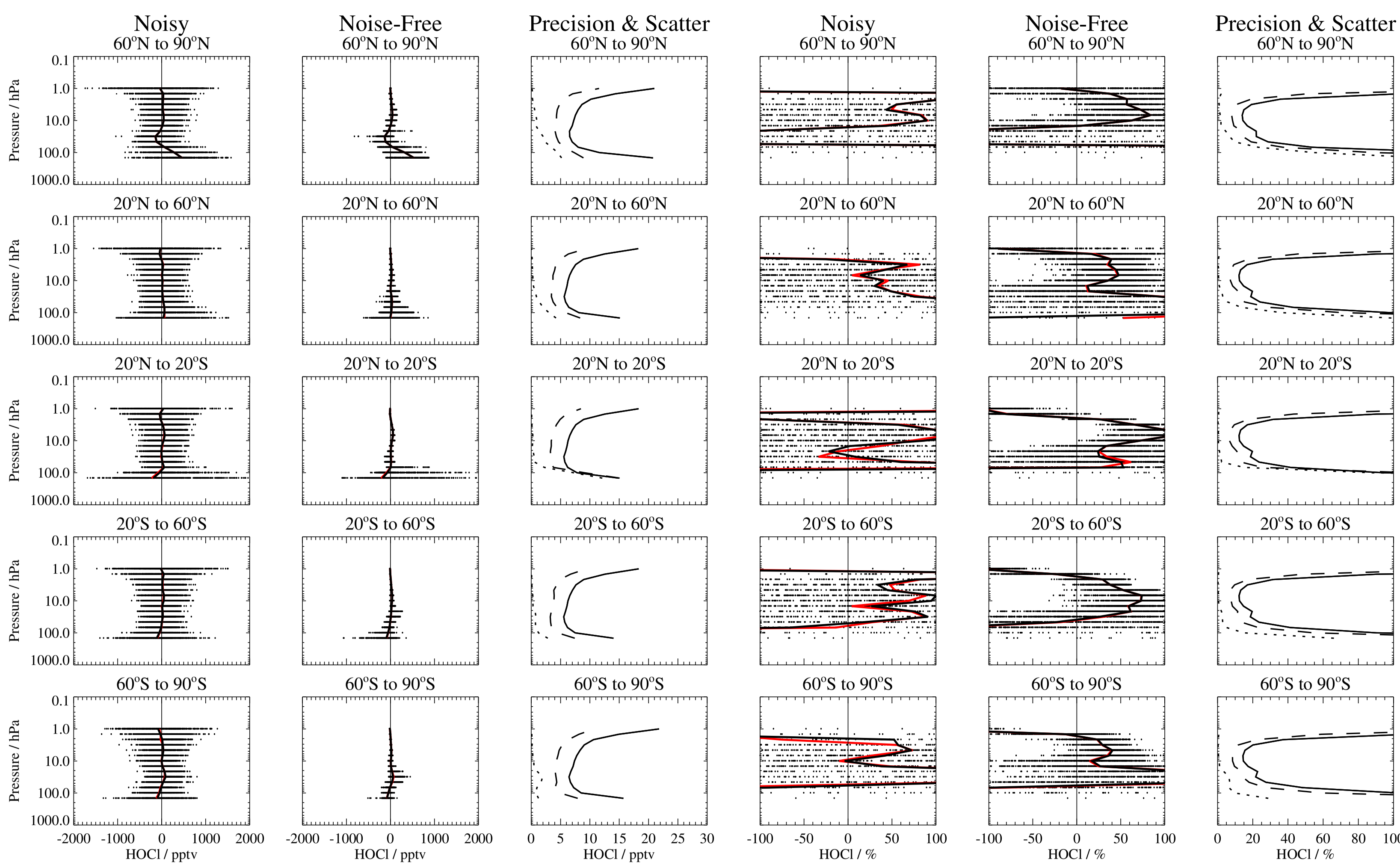


Figure 3.33: A summary of the v1.5 data quality for HOCl for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true HOCl as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of HOCl (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values.The estimated precision and observed scatter have been scaled here to correspond to those that would be expected from a monthly (30 day) zonal mean of HOCl in 5° wide latitude bins.

HOCl

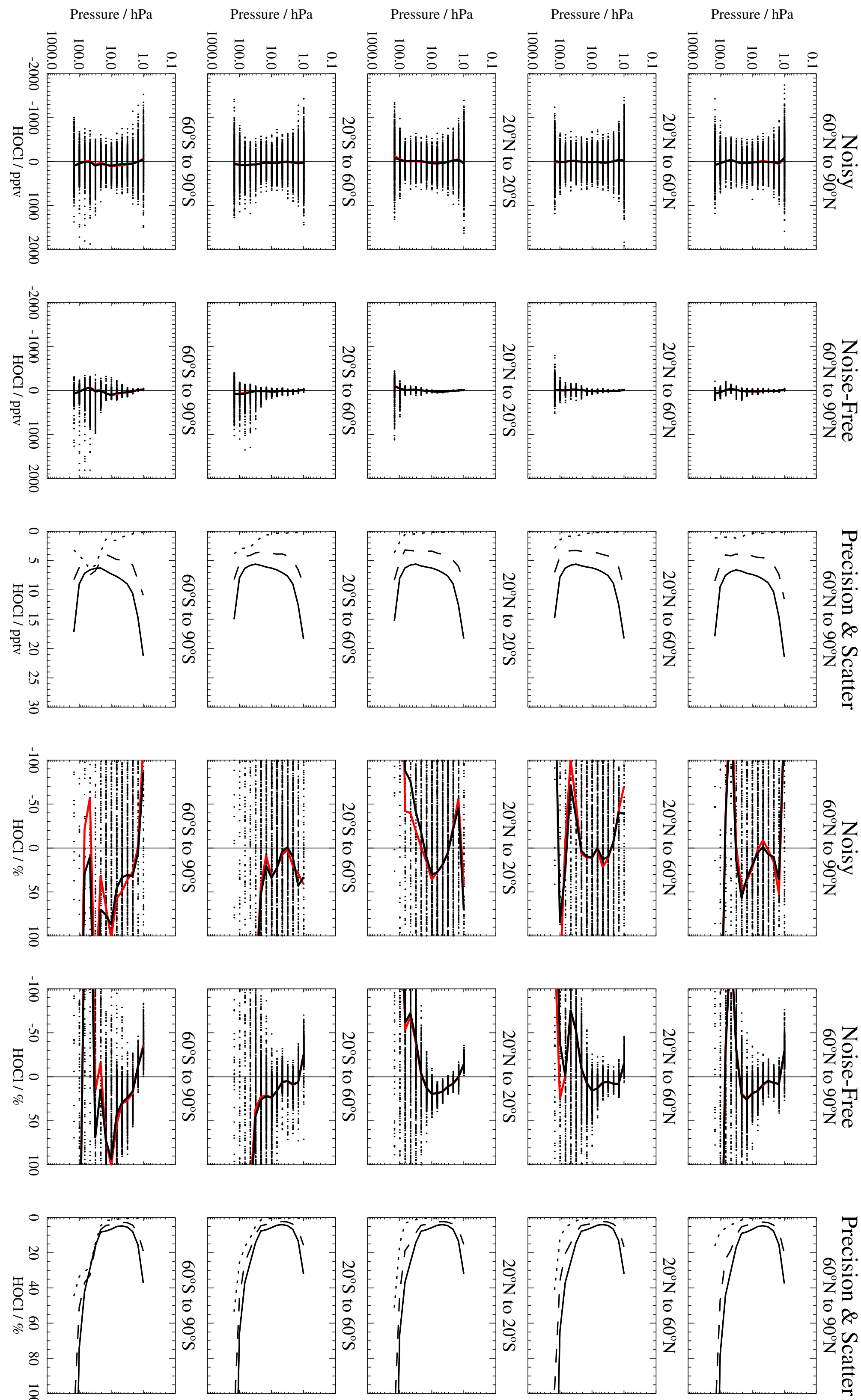


Figure 3.34: A summary of v1.5 data quality for HOCl as figure 3.33 for the `2000d276` test data set.

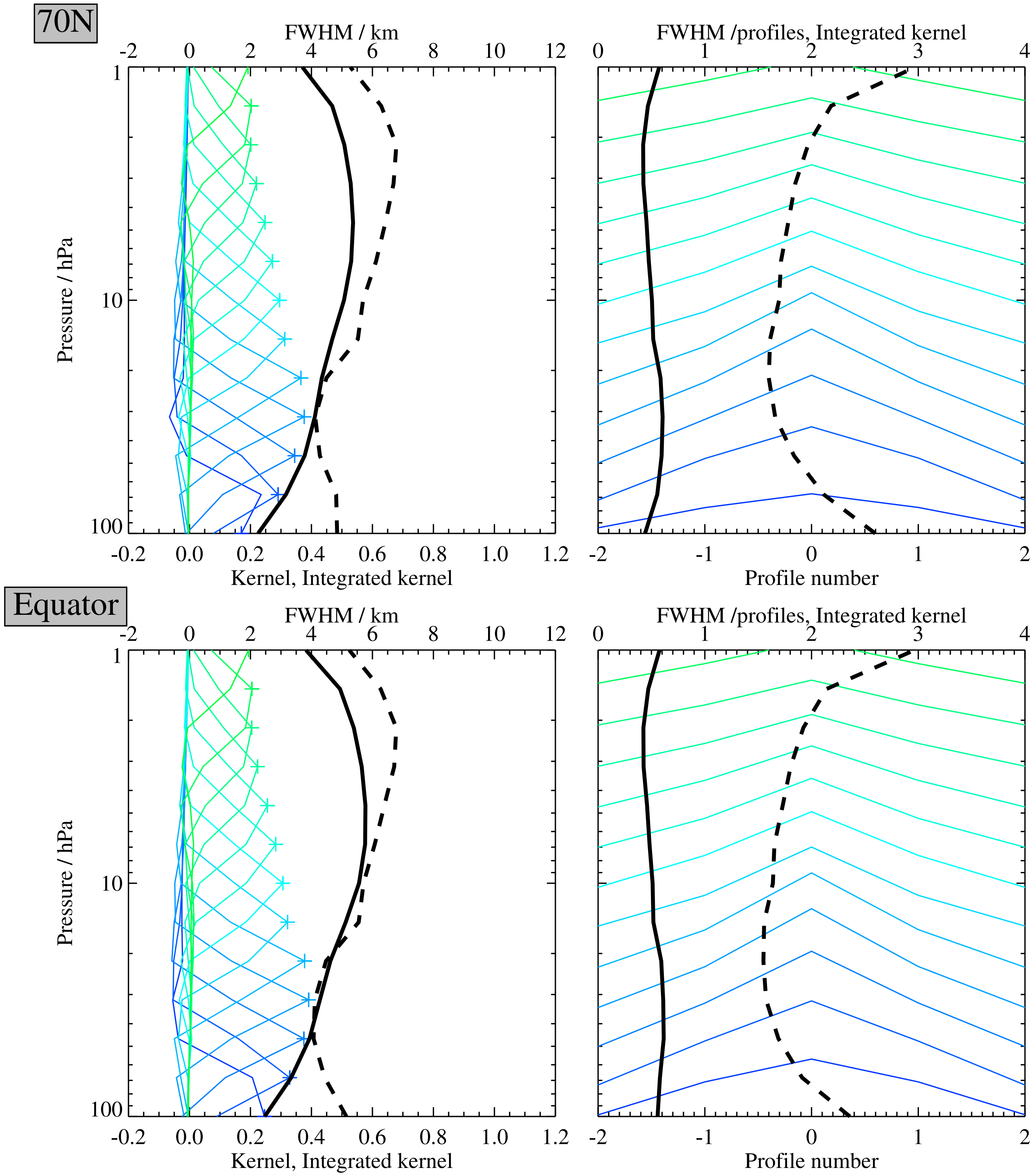


Figure 3.35: The left hand plots show the vertical averaging kernel for HOCl for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3). This is usually not an issue for the stratospheric heights recommended here, and given the large value chosen as *a priori* error (3 ppbv).

Averaging required: Given the noisy nature of the HOCl retrieval and its small abundance, averages such as monthly or bi-monthly zonal means will be required to reduce the noise to acceptably low values; some useful information may exist on shorter timescales, but caution is advised for such analyses.

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: There is currently no apparent need to discard profiles or profile portions where `Status` values indicate the existence/influence of clouds (see section 1.4).

Quality field: Profiles with a value of the `Quality` field (see section 1.4) less than 1.3 should not be used. This flag is an indication of occasional poor radiance fits; a very small fraction of HCl profiles (much less than 1%) will be discarded via this screening.

Artifacts

More investigations are needed to ascertain the nature of potential artifacts and the usefulness of this product, even in the currently limited recommended vertical range of 22 – 2.2 hPa.

Priorities for future data version(s)

Attempt to understand and reduce or remove the HOCl systematics (negative biases and oscillations) that are clearly evident for pressures outside the currently recommended vertical range, so that more useful atmospheric information can be obtained, especially for pressures larger than 22 hPa.

3.13 Ice Water Content

Swath name: IWC

Useful range: 215 – 68 hPa

Contact: Dong Wu, **Email:** <dwu@mls.jpl.nasa.gov>
Jonathan Jiang, **Email:** <jonathan@mls.jpl.nasa.gov>

The standard product for v1.5 IWC is retrieved from the 240-GHz cloud-induced radiances (T_{cir}) at 215 – 68 hPa.

Simulations and retrieval

For the simulation studies described at the start of this chapter, cloud-induced radiances (T_{cir}) were simulated using a 1D non-polarized radiative transfer model assuming Mie scattering, spherically-stratified atmosphere/-cloud layers, and a parameterized particle size distribution [McFarquhar and Heymsfield, 1997]. The resulting T_{cir} data were used to form an empirical relationship between the modeled T_{cir} and the IWC, for each pressure level.

This relationship forms the basis of the operational IWC retrieval, taking observed T_{cir} deduced from the MLS observations as input. At pressures smaller then 215 hPa, most clouds generate a positive T_{cir} and the linear portion of the relations is used for the IWC retrieval. T_{cir} is computed after the completion of Core+R2 retrieval phase from which realistic pressure, T, H_2O, O_3, HNO_3, and N_2O profiles are obtained. T_{cir} is defined as the radiance residual between measured and modeled radiances under the best-fit atmospheric state. Due to an error in the formation of the T_{cir} – IWC relation in the v1.5 software, a correction factor needs to be applied to the MLS IWC values, as detailed below.

MLS IWC represents an average over the volume of $\sim$200 $\times$ 7 $\times$ 3 km^3 (length, width, height) along the instrument line-of-sight. MLS sampling cannot resolve individual clouds, and therefore users are advised to exploit this dataset in statistical studies with a period of great than $\sim$5 days.

Artifacts

IWC

To correct the v1.5 IWC, the retrieved values should by multiplied by the numbers quoted in Table 3.1. This correction will make the MLS retrieval consistent with the IWC value predicted by the McFarquhar and Heymsfield [1997] parameterization.

Table 3.1: Estimated precision and correction factor for IWC

Pressure / hPa	Correction factor	Estimated precision / mg m^{-3}
215	0.25	4.4
178	0.22	2.2
147	0.23	1.6
121	0.20	0.6
100	0.20	0.4
82	0.20	0.4
68	0.20	0.4

The precision of v1.5 IWC, also tabulated in Table 3.1, is estimated based on the 3σ clear-sky standard deviation in Figure 3.36 and should be used instead of the precision values in the Level 2 IWC file. The accuracy remains to be assessed, it depends on the validity of the assumptions about cloud microphysics used in modeling the T_{cir}-IWC relations. The MLS sensitivity to IWC in the v1.5 product is degraded significantly above $\sim$50 mg m^{-3} because opaque clouds tend to 'saturate' the observations.

Data screening

Because T_{cir} can produce a non-zero, latitude-dependent bias, as shown in the resulting IWC in Figure 3.36, the user needs to remove this bias (orange line) on a daily basis and consider the 3σ standard deviation above the mean (red line) as the threshold for cloud detection. Such data screening has been performed by the MLS team through in offline processing, and the screened IWC data (blue points in Figure 3.36) can be obtained from MLS FTP site: `ftp://mls.jpl.nasa.gov/pub/outgoing/jonathan/mls_cld/`

Early results and validation

Preliminary studies show general agreement between MLS monthly IWC maps and those produced by climate models, where the differences are within model uncertainties [Li et al., 2005].

Priorities for future data version(s)

- Implement a non-linear T_{cir}-IWC relation for the IWC retrieval
- Improve the H_2O retrieval and continuum models to reduce the number of large negative IWC and biases.

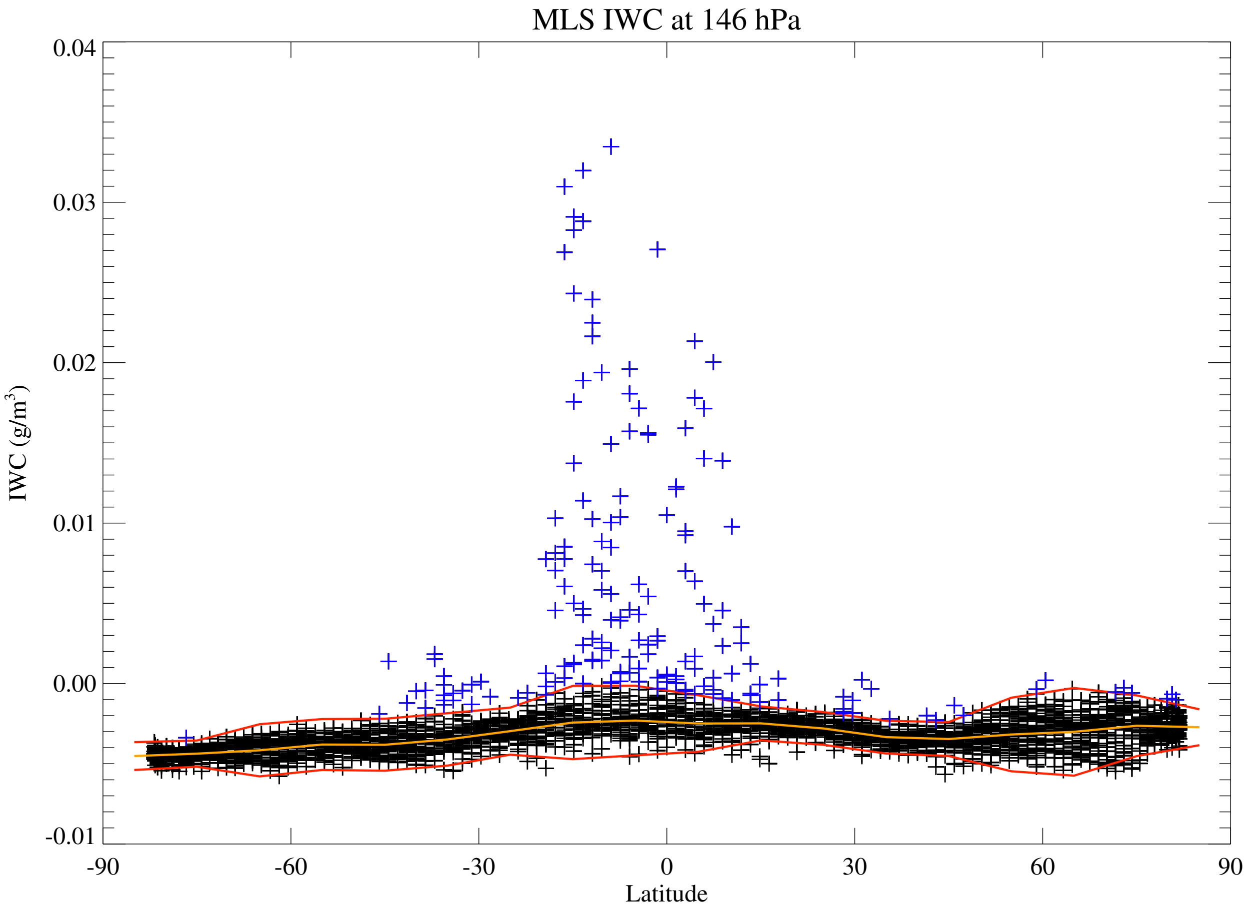


Figure 3.36: Example of the MLS 146-hPa IWC on 29 January 2005. The orange line is the mean bias of all the clear-sky measurements, which is computed iteratively by rejecting samples greater than 2σ standard deviation about the mean in each 10° latitude bin. The red lines are 3σ envelope about the mean. The values greater than the mean $+3\sigma$ (blue points) represent significant cloud IWC measurements.

IWC

3.14 Nitrous oxide

Swath name: `N2O`

Useful range: 100 – 0.1 hPa

Contact: Nathaniel Livesey, **Email:** `<livesey@mls.jpl.nasa.gov>`

The standard product for v1.5 N_2O is taken from the 640 GHz (Core+R4B) retrieval.

Simulations

The results of simulations are shown in figures 3.37 and 3.38. These show a reported precision for N_2O of around 20 ppbv in the mid-stratosphere, corresponding to about ~10%. The precision is poorer in the lowermost stratosphere and also worsens in the upper stratosphere. This reported precision overestimates the scatter seen in retrieval simulations by about 50%.

The simulations show that average biases are typically under ~10%, although individual points in the lower stratosphere can show biases as large as 100% in the winter polar vortex conditions.

Vertical resolution

Figure 3.39 shows that the vertical resolution for v1.5 N_2O is around 2 – 3 km in most of the stratosphere and lower mesosphere, worsening to 5 – 6 km in the lowermost stratosphere and at 0.1 hPa and above.

Early results and validation

- Initial comparisons with observations from the ACE instrument show mean biases of around −20%, and 40% scatter or better in the lower stratosphere.
- Comparisons of MLS N_2O observations with balloon borne observations are very encouraging, showing agreement within the expected levels of precision.

Data screening

Pressure range (100 – 0.1 hPa): Values outside this range are not recommended for use. In the upper stratosphere and lower mesosphere, v1.5 N_2O requires significant averaging (e.g., daily zonal means) for useful signals. Also see the note under 'Artifacts' for issues with N_2O at 100 – 68 hPa.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: An examination of several months of v1.5 data indicates that clouds do not have a significant impact (outside the noise) on N_2O profiles down to 100 hPa; there is currently no apparent need to discard profiles or profile portions where `Status` values indicate the existence/influence of clouds (see section 1.4).

Quality field: Profiles with a value of the `Quality` field (see section 1.4) less than 2.5 should not be used. This flag will throw out a few outliers (with very high or low abundances), but is mostly an indication of poor convergence and radiance fits, even for reasonable-looking profiles; a small fraction of N_2O profiles will be discarded via this screening.

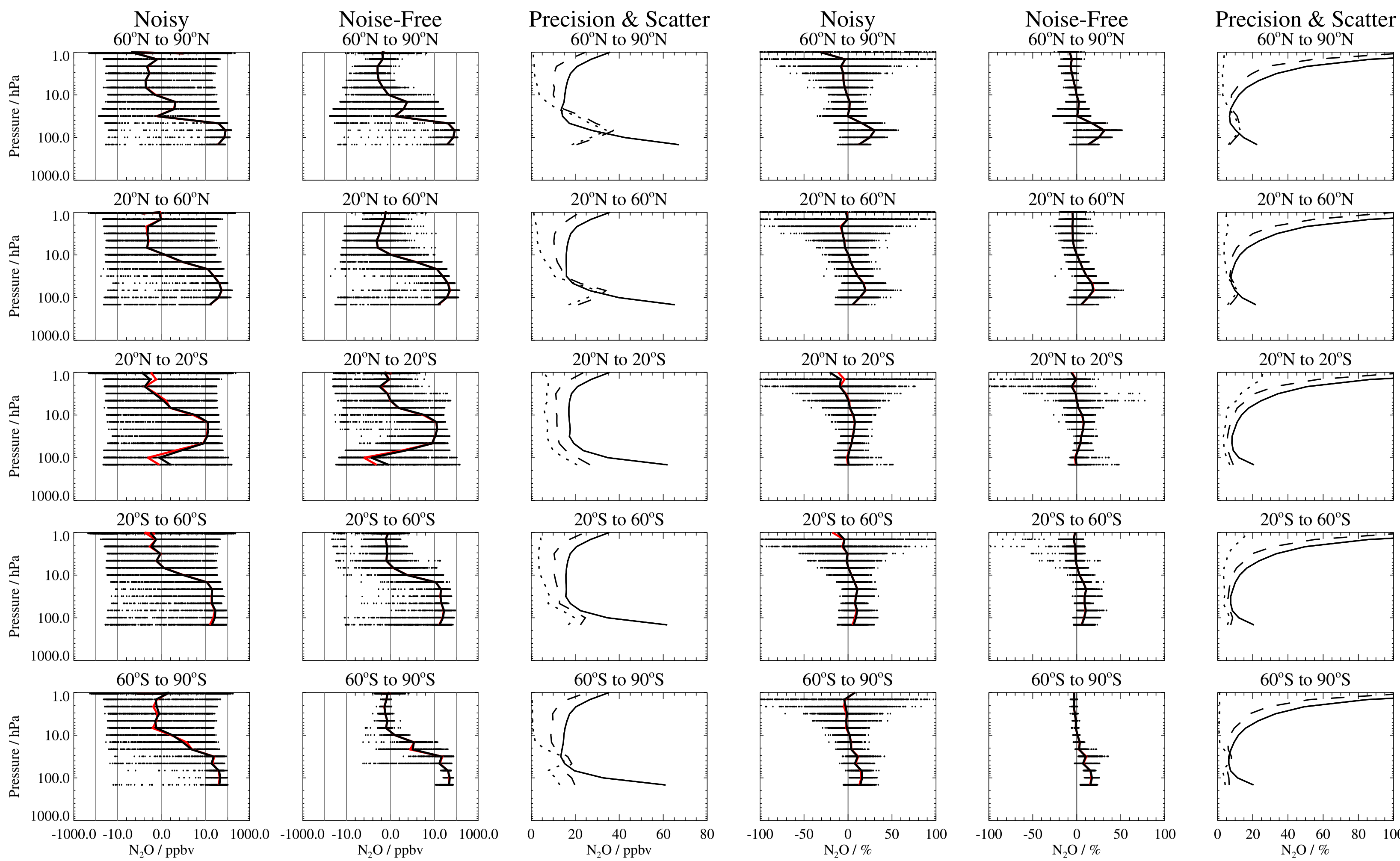


Figure 3.37: A summary of the v1.5 data quality for N_2O for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true N_2O as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of N_2O (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

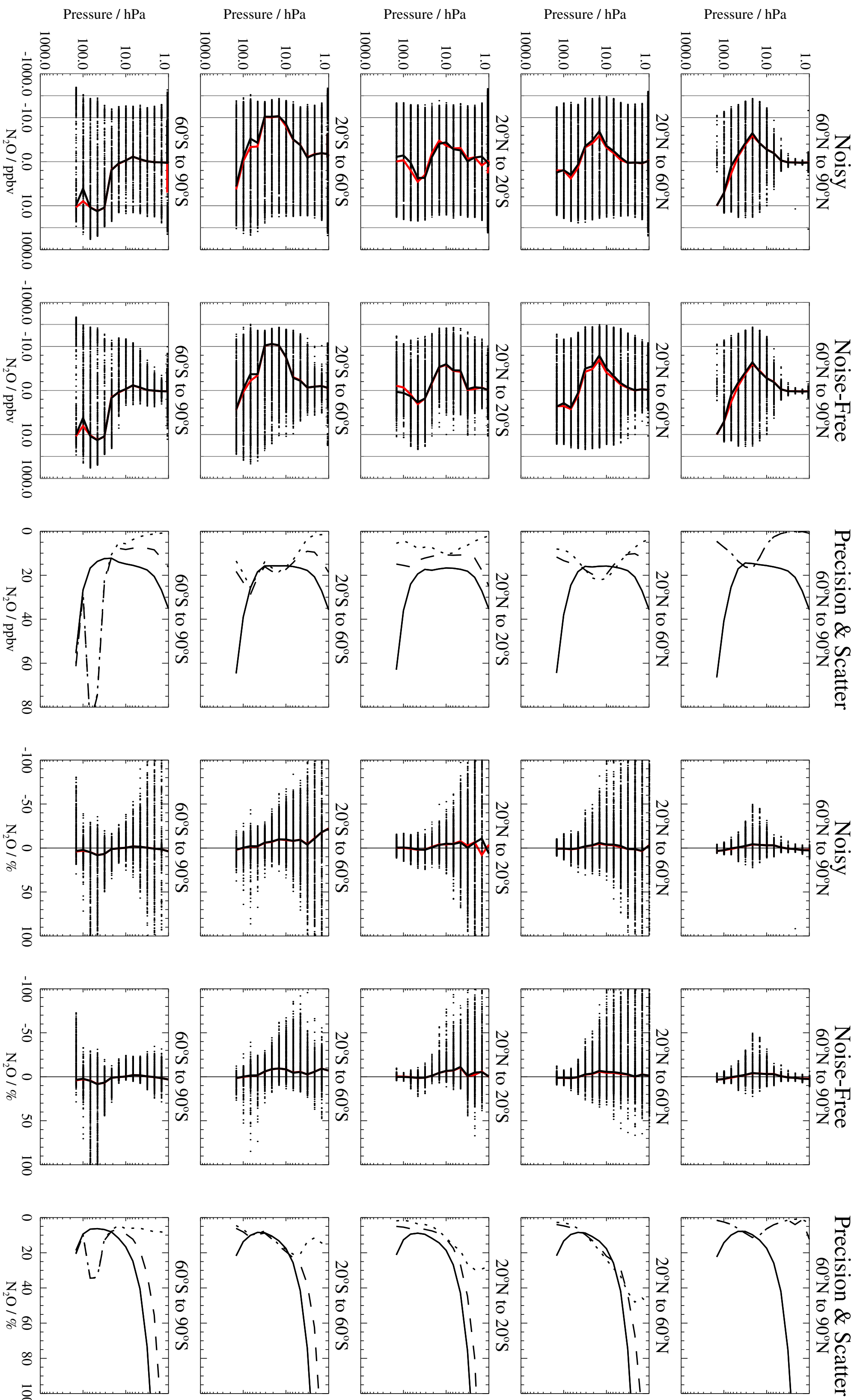


Figure 3.38: A summary of v1.5 data quality for N_2O as figure 3.37 for the 2000d276 test data set.

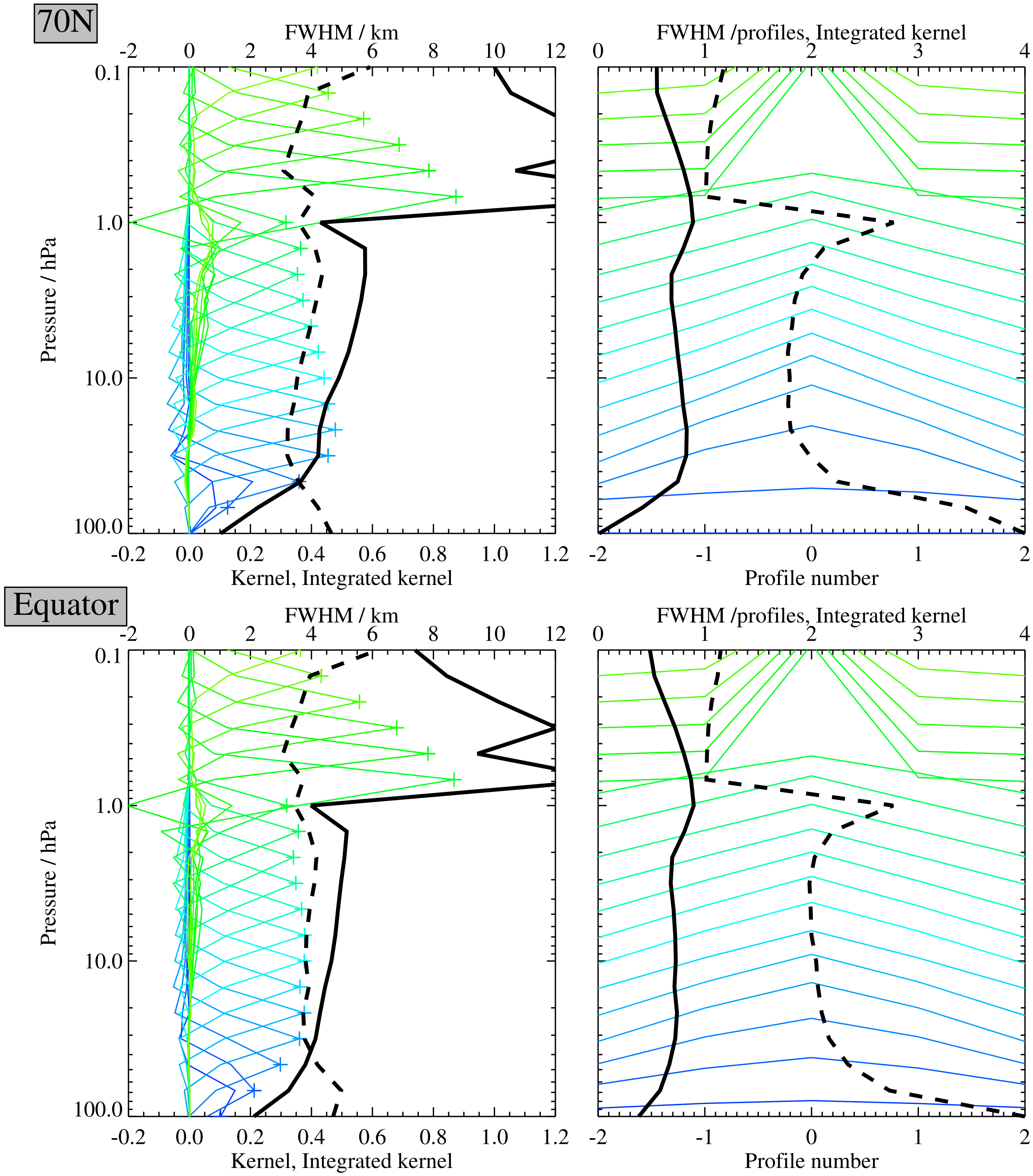


Figure 3.39: The left hand plots show the vertical averaging kernel for N_2O for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

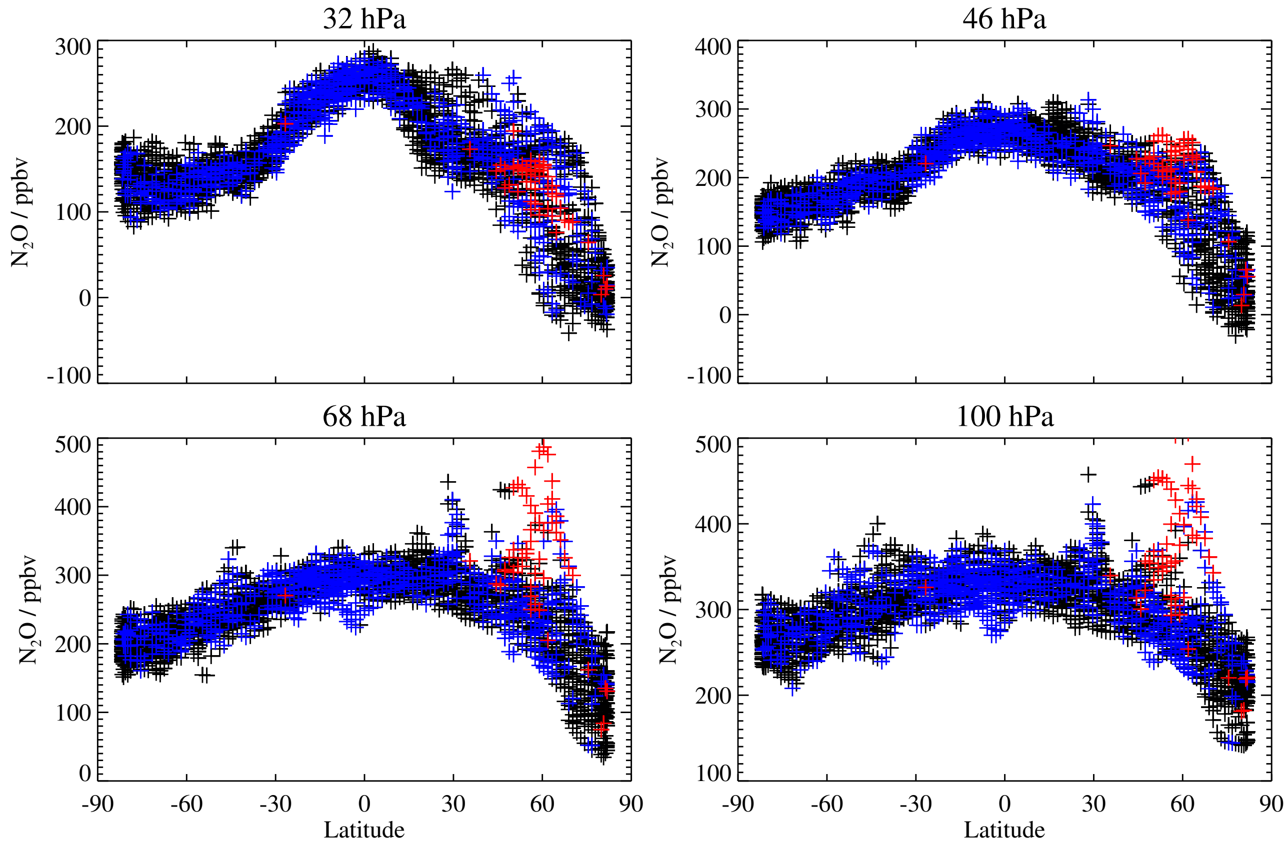


Figure 3.40: Sample N_2O results for 31st January 2005 as a function of latitude. The blue points are those flagged as possibly having been affected by clouds (clearly the impact is minimal). The red points have been flagged as having low quality at 100 and 68 hPa by an an off-line quality control algorithm.

Artifacts

N_2O data in the lower stratosphere (68 hPa and greater) polar vortex and near-vortex regions occasionally show high biases (see figure 3.40). A flag to screen out most of these values, based on independent data processing diagnostics (i.e., not involving comparisons of retrieved N_2O to *a priori* expectations) is available from `ftp://mls.jpl.nasa.gov/pub/outgoing/livesey/v1-5-n2omask/`, with individual files for each day. These simple ASCII data files, indicate good (`1`) or biased (`0`) profiles with one number for each `L2GP` N_2O profiles. Data at pressures less than 68 hPa are unaffected by this problem.

There are signs of poor convergence in some of the N_2O retrievals, resulting in sets of consecutive profiles that are temporally 'smooth'. These are successfully identified by applying the `Quality` screening described above.

Priorities for future data version(s)

The most important requirement for future versions is the elimination of the bias problem detailed above. This is thought to be due to badly converging retrievals. Possible improvements in the quality of the N_2O data at 147 hPa will also be studied. Retrievals of N_2O to pressures greater than 147 hPa *may* be possible in later versions, however, these data would be taken from the 190 GHz observations rather than the 640 GHz which currently forms the standard product.

N_2O

3.15 Ozone

Swath name: `O3`

Useful range: 215 – 0.46 hPa

Vertical resolution: 3 to 6 km

Contact: Lucien Froidevaux (stratosphere and above), **Email:** <lucien@mls.jpl.nasa.gov>
Mark Filipiak (troposphere), **Email:** <M.J.Filipiak@ed.ac.uk>

The standard product for version 1.5 O_3 is taken from the 240 GHz (Core+R3) retrieval. This product has the highest sensitivity down into the upper troposphere, as well as in the mesosphere. However, the mesosphere exhibits somewhat larger percent ozone differences between the 240 GHz band results and other MLS bands, as well as in comparisons between MLS and other datasets (see Froidevaux et al. [2005]). While we are conservatively recommending 0.46 hPa as an upper limit for detailed analyses that require very accurate results, there is clearly good O_3 sensitivity into the upper mesosphere. For example, this region at high latitudes has shown the impact of solar proton events on the MLS O_3 distribution (as well as in the other radiometers' ozone retrievals).

Simulations

Stratosphere and above: Retrieval simulations indicate that average biases are small over the vertical range recommended above, with overall accuracy (closure) of better than $\sim$1%, not a major error source, and there is excellent tracking between the simulated retrieval results and the true input profiles. An iterative full forward model is used for increased accuracy over a broad altitude range. A small (a few %) negative bias is sometimes seen in the lower mesosphere. The estimated precision for stratospheric ozone compares well with the RMS scatter about the truth.
Upper troposphere: Simulations indicate good closure for O_3 in the upper troposphere, typically to better than $\sim$10%. Larger percentage biases (30–40%) are sometimes apparent in the 200–300 hPa range. Based on these simulations (and plots not shown here), the impact of clouds (those thick enough to affect the MLS retrievals significantly) can be large in the tropical upper troposphere, especially at 215 hPa and higher pressures. The scatter is larger than the estimated precision in a few regions, most notably the tropical upper troposphere, where the minimum estimated precision of $\sim$20 ppbv is overestimated by about a factor of two. Tropospheric O_3 will often require some averaging to give useful information, but isolated incursions of high O_3 from the stratosphere should be measurable.

Vertical resolution

Based on Figure 3.43, the vertical resolution for the standard O_3 product is $\sim$3 km in the upper troposphere and lower stratosphere, but degrades to $\sim$4 km at 215 hPa and 6 km in the mesosphere.

Early results and validation

Stratosphere and above: The estimated single-profile precision reported by the Level 2 software typically varies from $\sim$0.2 to 0.4 ppmv (or 2 to 15 %) from the mid-stratosphere to the lower mesosphere. The observed scatter in the data, evaluated in a narrow latitude band centered around the equator where atmospheric variability is expected to be small, tends to be slightly larger than these values. This scatter is larger than the estimated precision by $\sim$30% near the ozone peak, and by a factor of more than two near 100 hPa. Some of this may be caused by atmospheric variability, as well as by smoothing constraints (used for the a priori profile). The early O_3 comparisons [Froidevaux et al., 2005] indicate overall agreement at roughly the 5 – 10 % level with

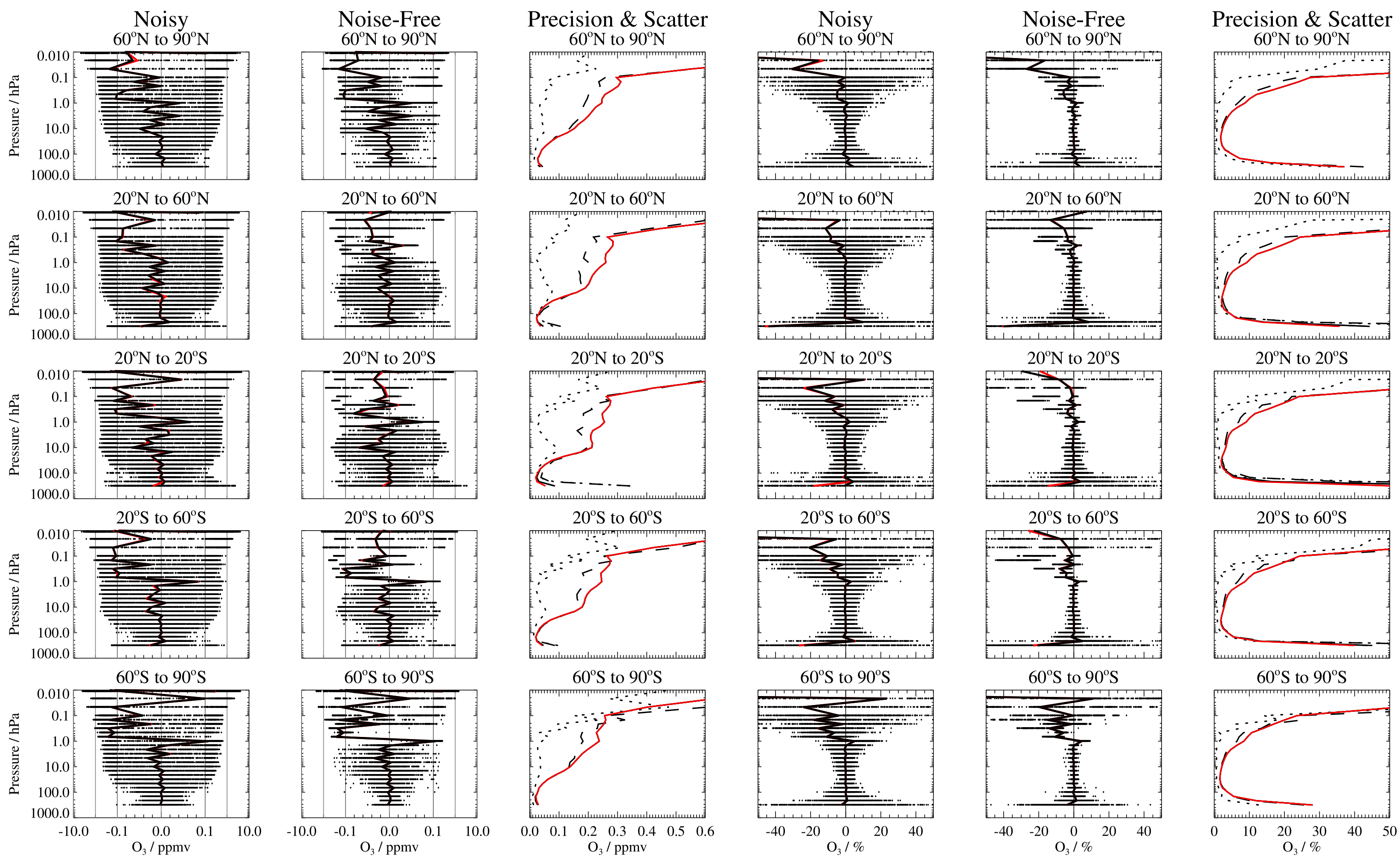


Figure 3.41: A summary of the v1.5 data quality for O_3 for the `1996d051` test data set. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved and true O_3 as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the mean estimated precision of individual profiles of O_3 (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. The remaining three columns show the same information as in the first three columns in the form of a percentage of the true values. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

O_3

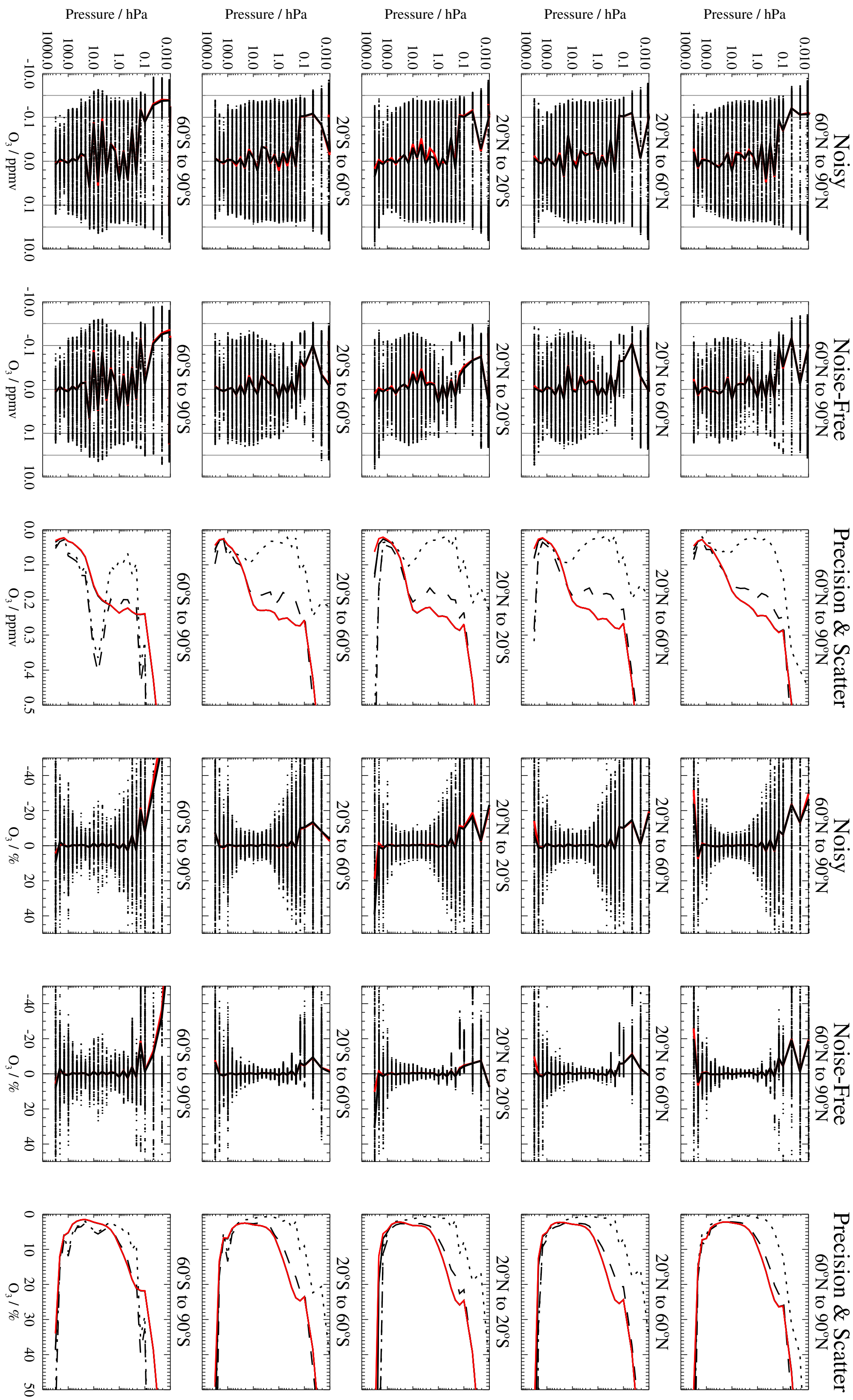


Figure 3.42: A summary of v1.5 data quality for O_3 as figure 3.41 for the 2000d276 test data set.

O3

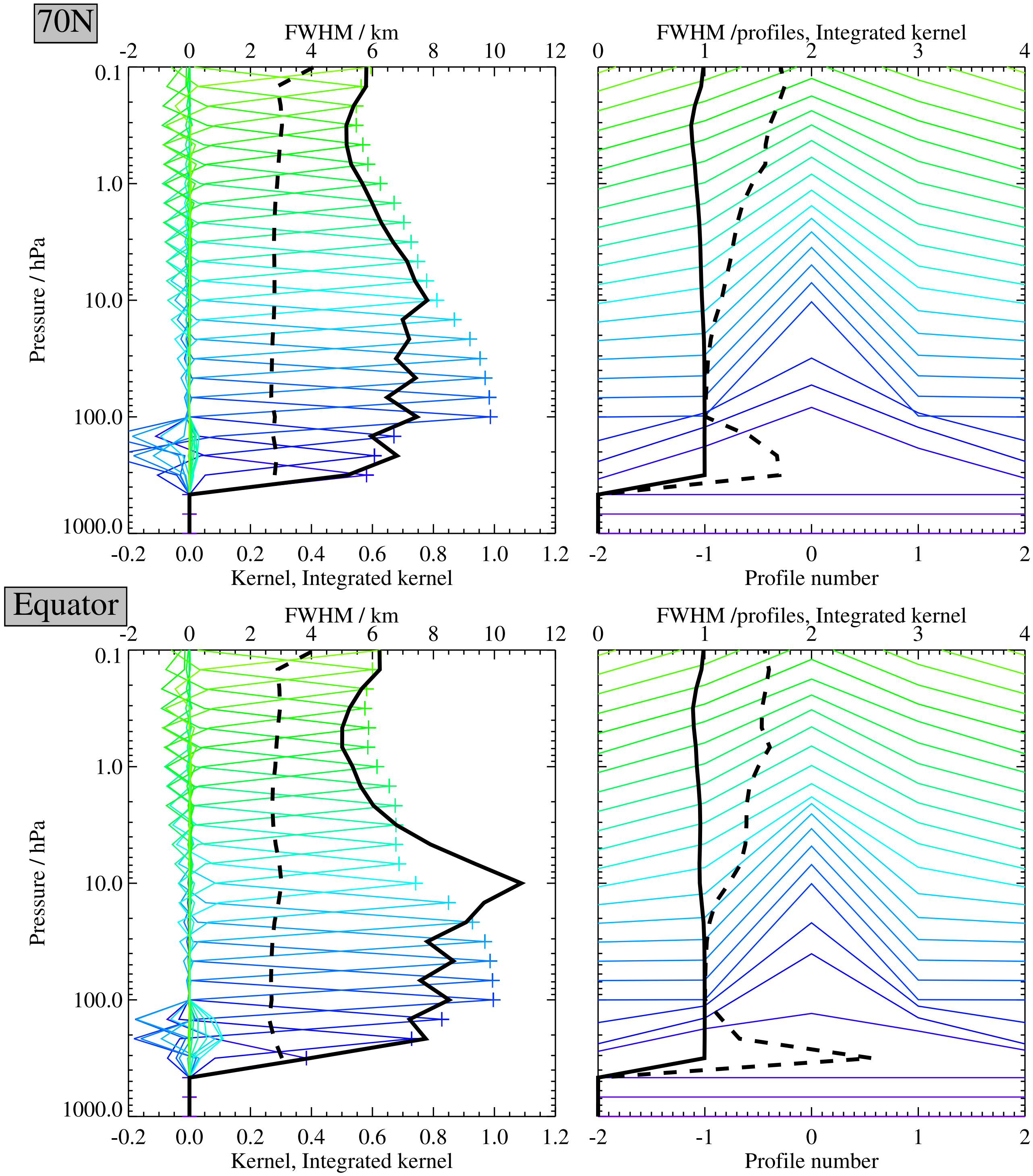


Figure 3.43: The left hand plots show the vertical averaging kernel for O_3 for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

stratospheric profiles from SAGE II, HALOE, POAM III, and ACE. MLS ozone values tend to be slightly higher than the occultation datasets in the lower stratosphere, and slightly low in the upper stratosphere, but the degree of 'tilt' in this slope of the average differences changes from one comparison to the next, indicating that there are also differences between the occultation datasets themselves (see Froidevaux et al. [2005] for more details). The standard MLS product leads to a better overall match versus the other satellite measurements than do O_3 products from the other MLS radiometers, but the 'sloping' nature of many of these differences is not a feature of the standard MLS product alone. However, the other MLS ozone products tend to have smaller values for lower mesospheric O_3 than the standard O_3 product; this may be in part because of issues relating to the narrower spectral channels (digital autocorrelator spectrometers or DACs) used for the 240 GHz band retrievals. Any overestimate in the mesosphere could lead to some underestimate near 1 hPa, but this remains to be investigated. More care will be needed in these comparisons in terms of the sunrise and sunset differences and the most appropriate MLS comparisons; moreover, there are varying degrees of correction in the occultation measurements for the inhomogeneity in the line-of-sight for this region, where ozone changes quickly from day to night, and this probably plays a role as well.

We have also compared the MLS ozone data to some ozonesonde measurements as well as the Ft. Sumner 2004 Fall balloon-borne ozone measurements, and found overall good agreement, given the various error bars. We expect to get more detailed statistical information for the lower stratosphere from a more systematic approach in terms of MLS versus ozonesonde profiles.

Atmospheric variability is generally very well matched between MLS and the other satellite observations. There are also many instances where variations near the NH vortex edge or in and out of the vortex are well tracked by both MLS and the other satellite measurements, based on plots of matched profiles on individual days.

Upper troposphere: Limited comparisons with SHADOZ ozonesonde data in the tropics indicate that MLS ozone data have a positive bias (sometimes by up to 100%) at 215 hPa.

Data screening

Pressure range (215 – 0.46 hPa): Data outside this range are not recommended for use, although the top level is a conservative value, as mentioned above.

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: Data in the troposphere should not be used if the status is 'questionable' (`Status` bit 1 set), see section 1.4. This signals profiles affected by clouds, according to the MLS cloud detection scheme, and leads to radiometer 3 radiances being deleted from the retrievals; we recommend that data at pressures smaller than 100 hPa still be used in this case. This can eliminate ~5 – 10% of the MLS data, globally, but most of this is in the tropics, where 10 – 15% of the tropospheric profiles may be screened out. A less conservative flag may be possible in future recommendations, but we do not have a robust scheme worked out for this yet.

Quality flag: Profiles with a value of the `Quality` field (see section 1.4) less than 0.10 should not be used, this is an indication of poor radiance fits, even for reasonable-looking profiles. A very small fraction of O_3 profiles (much less than 1%) will be discarded via this screening.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Artifacts

Upper stratosphere and lower mesosphere: Some caution should be exercised in this region, since differences between MLS and occultation datasets becomes larger there. Reasons for these larger percent differences may include issues with this radiometer’s retrievals, time of day issues, and/or occultation measurement issues in regions of strong gradients during twilight, and will require further investigation.

215 hPa: High biases exist at 215 hPa for low latitudes, even if daily to weekly maps at this pressure level show reasonable morphology, e.g., versus results from the GEOS-CHEM model. These biases require further investigation.

Columns: Users of the column ozone data from the MLS Level 2 files should be aware that these values and any other such column values have some artifacts, especially at high latitudes. This seems to be caused by limitations in the current (MLS software) calculations of tropopause pressure, as described in section 1.7; the use of alternative values for this parameter is required for better results.

Priorities for future data version(s)

- Improve the upper tropospheric data: mainly by reducing/eliminating the low latitude biases at 215 hPa (and at 316 hPa), and extending the useful range to 316 hPa, if possible.
- Better characterize biases versus satellite occultation datasets in the uppermost stratosphere and lower mesosphere, with a goal of reducing this bias.
- Recommend somewhat better screening methods for cloud effects and the quality parameter (e.g., by looking in more detail at radiance fits versus altitude), if possible.

3.16 The hydroxyl radical

Swath name: `OH`

Useful range: 46 – 0.2 hPa

Contact: Herbert Pickett, **Email:** `<hmp@mls.jpl.nasa.gov>`

The standard product for version 1.5 OH is taken from the 2.5 THz (Core+R5) retrieval.

Simulations

Simulations (see the left two columns in Figures 3.44 and 3.45) indicate closure for OH to better than 10 % of the daytime (ascending) typical OH values. The scatter shown in the right column in these figures for the noise-free simulations at all latitudes is significantly smaller than the precision. The scatter in the noisy simulations is comparable to the estimated precision.

Vertical resolution

Based on Figure 3.46, the vertical resolution for OH is ∼3 km in the stratosphere, and degrades to 5 – 6 km above 0.1 hPa up to the top recommended level of 0.001 hPa.

Early results and validation

OH is being validated using the balloon-borne FIRS-2 and BOH instruments. Preliminary results for September 23, 2004 for the region of Ft. Sumner, NM show excellent agreement between the FIRS-2, BOH, and MLS instruments [Pickett et al., 2005].

Retrieved concentrations of OH in the mesosphere are often negative with estimated precisions that are much smaller than the size of the negative excursion. These negative concentrations are likely due to subtle inadequacies in the forward model or due to non-linearities in the retrieval. Use of day-night differences does not help in this case. Positive concentrations in levels adjacent to negative concentrations are likely to overestimate the actual OH concentration.

Data screening

Pressure range (46 – 0.002 hPa): Values outside this range are not recommended for use. Day - night differences are recommended in the range of 46 – 10 hPa.

Test for poor convergence: The version 1.51 retrievals for OH generate poorly converged profiles about ∼15 % of the time. This can have a significant impact on zonal means, as the poorly converged profiles cluster in latitude. The poorly converged retrievals can be recognized because the OH fields are 'too smooth'. This situation is not automatically recognized by the Level 2 software, and needs to be identified in off-line studies, see below for more information.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, to avoid too strong an *a priori* influence (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Clouds: Within the recommended pressure range, clouds should not have any effect of OH concentration. There is currently no need to discard profiles or profile portions where `Status` values indicate the existence/influence of clouds (see section 1.4).

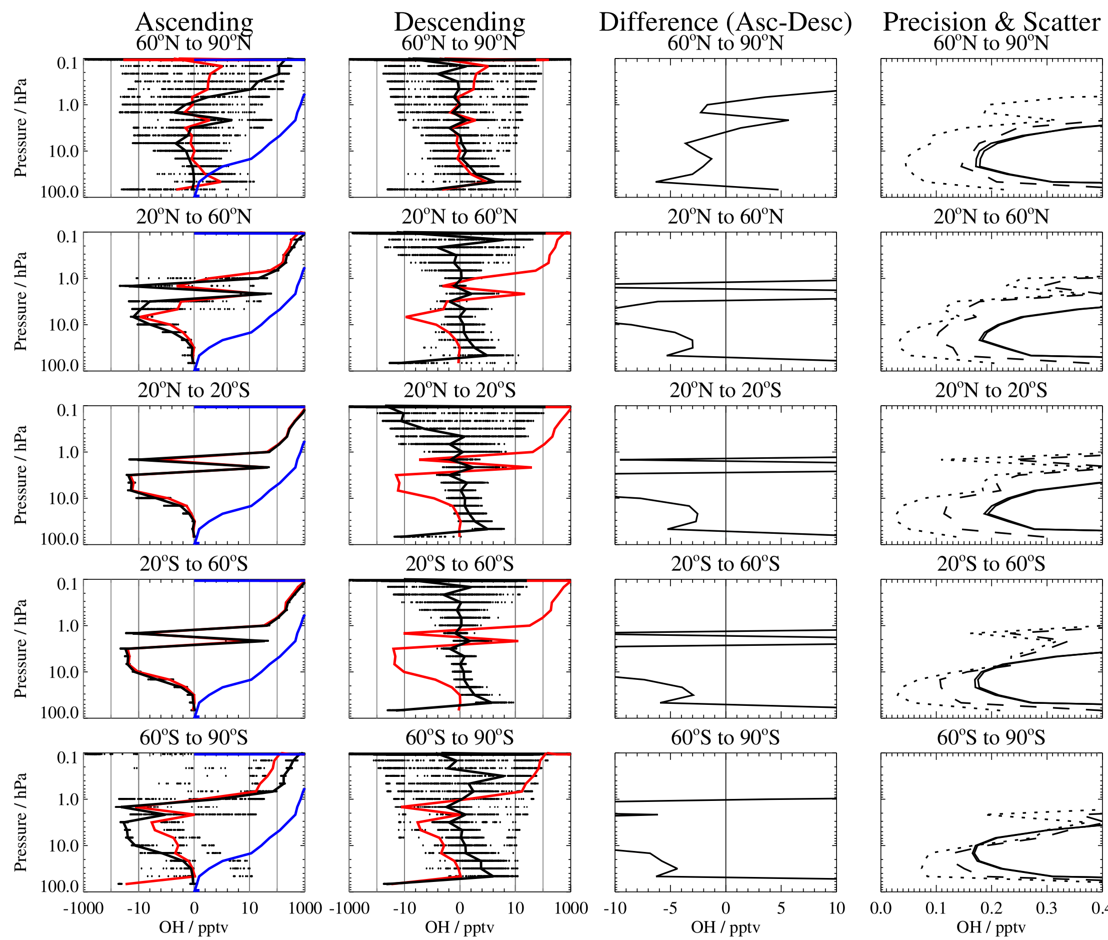


Figure 3.44: A summary of the v1.5 data quality for OH for the `1996d051` test dataset. Each row of panels represents a broad latitude bin. The first two columns show, for the noise-free case, the differences between the retrieved and true OH as a function of pressure for the ascending and descending phases of the Aura orbit (corresponding to mainly day and mainly night observations respectively). Also shown is a solid line that indicates the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The third column shows the difference in the median biases (solid black lines in previous columns) between the ascending and descending side. The fourth column shows the mean estimated precision of monthly zonal means of OH in 5° wide latitude bins (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases, scaled to correspond to the 'scatter' that would be expected in the monthly zonal means. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.The blue line in the first column of plots indicates a typical abundance of OH for reference.

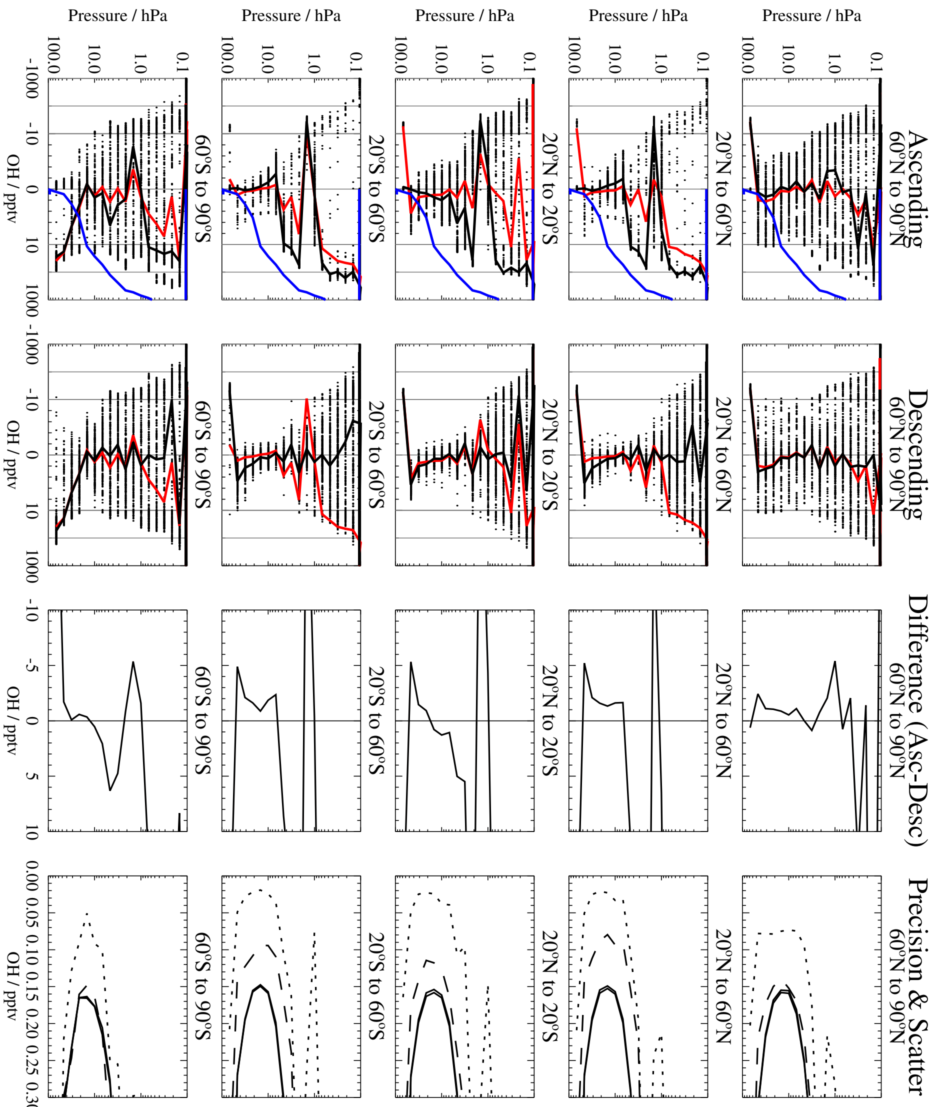


Figure 3.45: A summary of v1.5 data quality for OH as figure 3.44 for the 2000d276 test data set.

OH

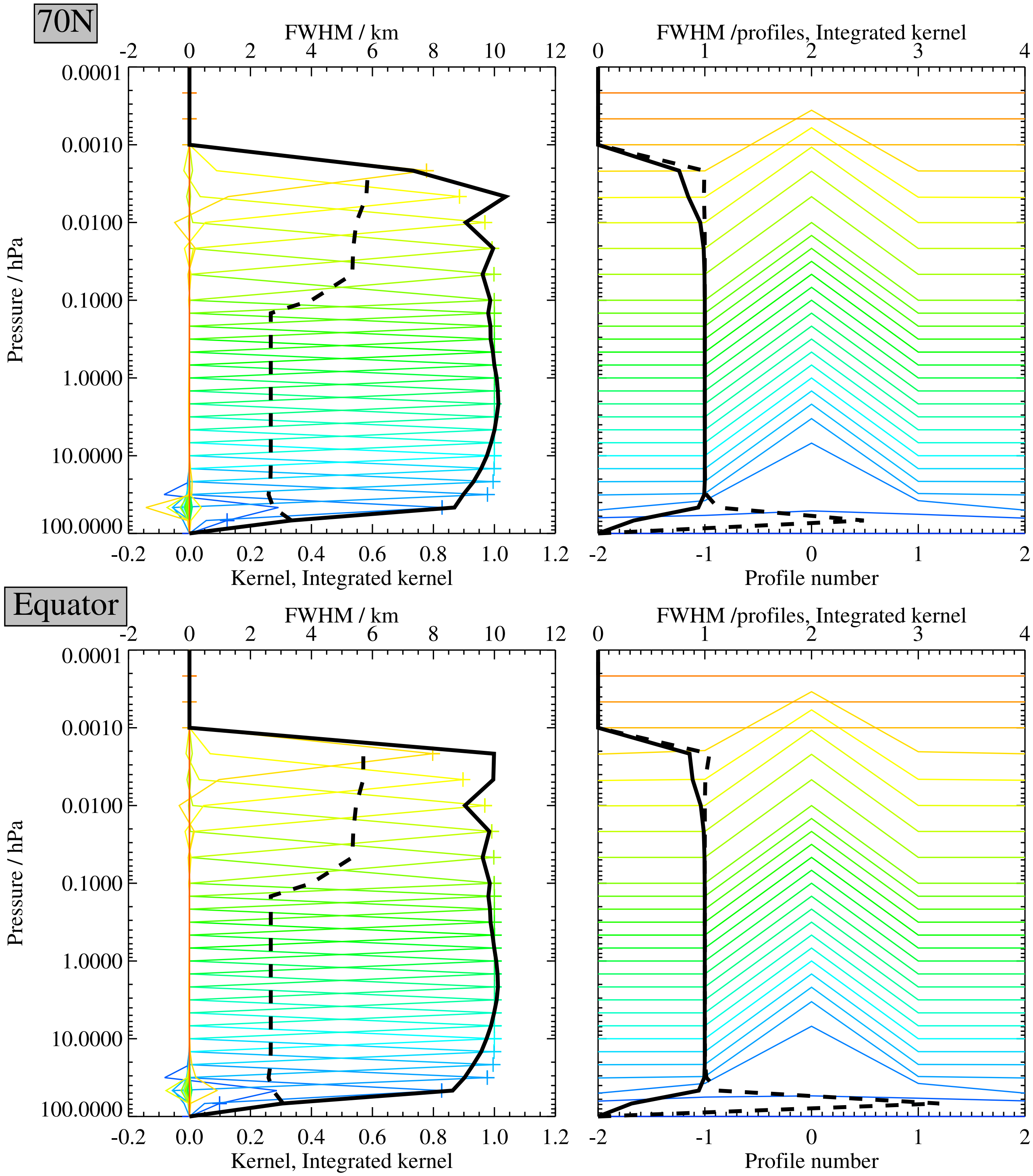


Figure 3.46: The left hand plots show the vertical averaging kernel for OH for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

Quality field: Profiles with a value of the `Quality` field (see section 1.4) less than 0.5 should not be used. This flag is mostly an indication of poor radiance fits, even for reasonable-looking profiles; a very small fraction of OH profiles (much less than 1%) will be discarded via this screening.

Additional filtering required for OH observations

Studies of v1.5 data have indicated that the quality flags shown here can miss cases where adequate convergence has been achieved in retrievals. The MLS profiles are retrieved in 'chunks' typically of ten profiles (shorter chunks are found at day boundaries and adjacent to data interruptions). The symptom of this poor convergence is that the along-track variability within a chunk is 'too smooth' when compared to the amounts of noise predicted. These bad retrievals are particularly prevalent for the OH standard product.

To recognize these situations, users should look at the scatter in the retrieved OH data about a simple linear fit within each chunk (i.e., for all profiles that share the same `ChunkNumber` field in the `L2GP` files), for each given pressure level. The coefficients of the fit are given by

$$a = \frac{1}{10}\sum_{j=0}^{9} C_{p,k+j} \tag{3.5}$$

$$b = \frac{1}{82.5}\sum_{j=0}^{9}(j-4.5)C_{p,k+j} \tag{3.6}$$

where k is the beginning index for a given chunk. The scatter about the fit can be compared to that expected by calculating

$$r = \sqrt{\frac{1}{10}\sum_{j=0}^{9}\left[\frac{C_{p,j+k}-a-b(j-4.5)}{\sigma_{p,k+j}}\right]^2} \tag{3.7}$$

where $\sigma_{p,k+j}$ is the reported precision for concentration $C_{p,k+j}$. When $r < 0.05$, the retrieval for this chunk and pressure level is likely to be incompletely converged.

Artifacts

- Concentrations in the mesosphere can be negative with estimated precisions that are much smaller than the size of the negative excursion. Altitudes adjacent to these negative excursions are likely to be influenced due to correlations.
- Proper data screening is essential. Otherwise, poorly converged retrievals can have a significant impact on overall results.

Priorities for future data version(s)

- Eliminate or reduce the retrieval convergence problem.
- Make sure poorly converged retrievals are flagged appropriately.
- Use logarithmic concentration basis to force concentrations to be positive and investigate cause of negative concentrations.
- Improve OH at pressures smaller than 0.2 hPa.

3.17 Relative Humidity with respect to Ice

Swath name: `RHI`

Useful range: 316 – 0.1 hPa

Vertical resolution: 7 to 8 km

Contact: William Read, **Email:** `<bill@mls.jpl.nasa.gov>`

RHi is relative humidity with respect to ice. It is a derived product from the standard products of water vapor and temperature using the Goff-Gratch formula.

Data screening

The same screening criteria that is to be applied to H_2O also applies to RHi, (see the discussion starting on page 45). Unfortunately, the sign of the uncertainty field in RHi has not been correctly set in the RHi file for v1.5, therefore the user must consult the H_2O and Temperature files for this information. If either (or both) has a negative value for precision, then the corresponding RHi profile must not be used. The `Status` and `Quality` fields are copies of those from the H_2O product. However, the `Status` and `Quality` information for the Temperature product should also be considered as part of any data screening, as described starting on page 105.

Artifacts

The vertical resolution of the temperature product is 7–8 km, much poorer than for H_2O. Therefore RHi has poorer vertical resolution than its associated H_2O product.

Priorities for future data version(s)

- Improve the vertical resolution of the Temperature product.
- Compute RHi on 12 levels per decade pressure (double the current sampling) in the troposphere and lower stratosphere from the 12 levels per decade H_2O product.

3.18 Temperature

Swath name: `Temperature`

Useful range: 316 – 0.001 hPa

Vertical resolution: 7 – 8 km from 316 to 100 hPa, 4 km at 31 – 6.8 hPa, 6 km at 1 hPa, 9 km at 0.1 hPa

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The standard product for temperature is taken for the Core retrieval (118 GHz only) from 316 – 1.41 hPa and from the Core+R2A (118 GHz and 190 GHz) retrieval from 1 hPa to 0.001 hPa.

Preliminary validation shows Core+R2A temperature to be somewhat more prone to vertical oscillation than Core temperature at the lowest retrieval levels (316 – 100 hPa), however its superior vertical resolution (∼5.5 km vs. ∼8 km) may make it preferable for some uses. There is little to choose between these phases in the mid stratosphere. Core+R3 temperature is significantly more succeptible to vertical oscillation and has persistent biases in the lowest retrieval levels.

Simulations

Simulations (see Figures 3.47 and 3.48) show retrieval scatter typically comparable to, or slightly less than the estimated retrieval precision throughout the stratosphere, with values generally less than 1 K, and with a minimum of approximately 0.5 K in the lower stratosphere. Performance is poorer in the winter polar bin for both simulation days. Simulations also show retrieval instability leading to vertical oscillations. There is a vertical oscillation near 1 hPa in the `1996d051` simulation with peak-to-peak magnitude of 2 – 4 K and vertical wavelength of 2/3 of a decade of pressure and a similar oscillation in the southern (winter) polar bin of the `2000d276` simulation below 10 hPa. At levels above 0.1 hPa, the `2000d276` retrieval becomes unstable, with a peak-to-peak oscillation as large as 25 K in the southern polar bin.

Vertical oscillations in Core+R2 and Core+R3 temperatures in the stratosphere and upper troposphere are larger, leading to the use of Core Temperature as the standard v1.5 product at these levels despite its poorer vertical resolution.

Vertical resolution

Based upon Figure 3.49, the vertical resolution for the standard Temperature product is 7 – 8 km from 316 to 100 hPa, 4 km at 31 – 6.8 hPa, 6 km at 1 hPa, and 9 km at 0.1 hPa. Improved vertical resolution over 316 – 100 hPa is given by Core+R2A (∼5.5 km) and Core+R3 (∼4.5 km), but at the cost of vertical oscillation and biases, particularly in Core+R3 temperature, (see section A.10), motivating the choice of Core Temperature as the standard product in this version of the software.

Early results and validation

Initial comparisons with ACE, HALOE and CHAMP measurements and with the GEOS-4 model [Froidevaux et al., 2005] suggest that MLS temperature has a warm bias of 1 – 2 K in the lower stratosphere (100 – 14.7 hPa). The 10 hPa level has a 2 – 4 K warm bias, and higher in the stratosphere there is an oscillation in the biases, with 6.8 – 4.6 hPa warm by 1 K, 3.16 – 2.15 hPa warm by 3 K and 1.47 – 1.0 hPa having bias near zero.

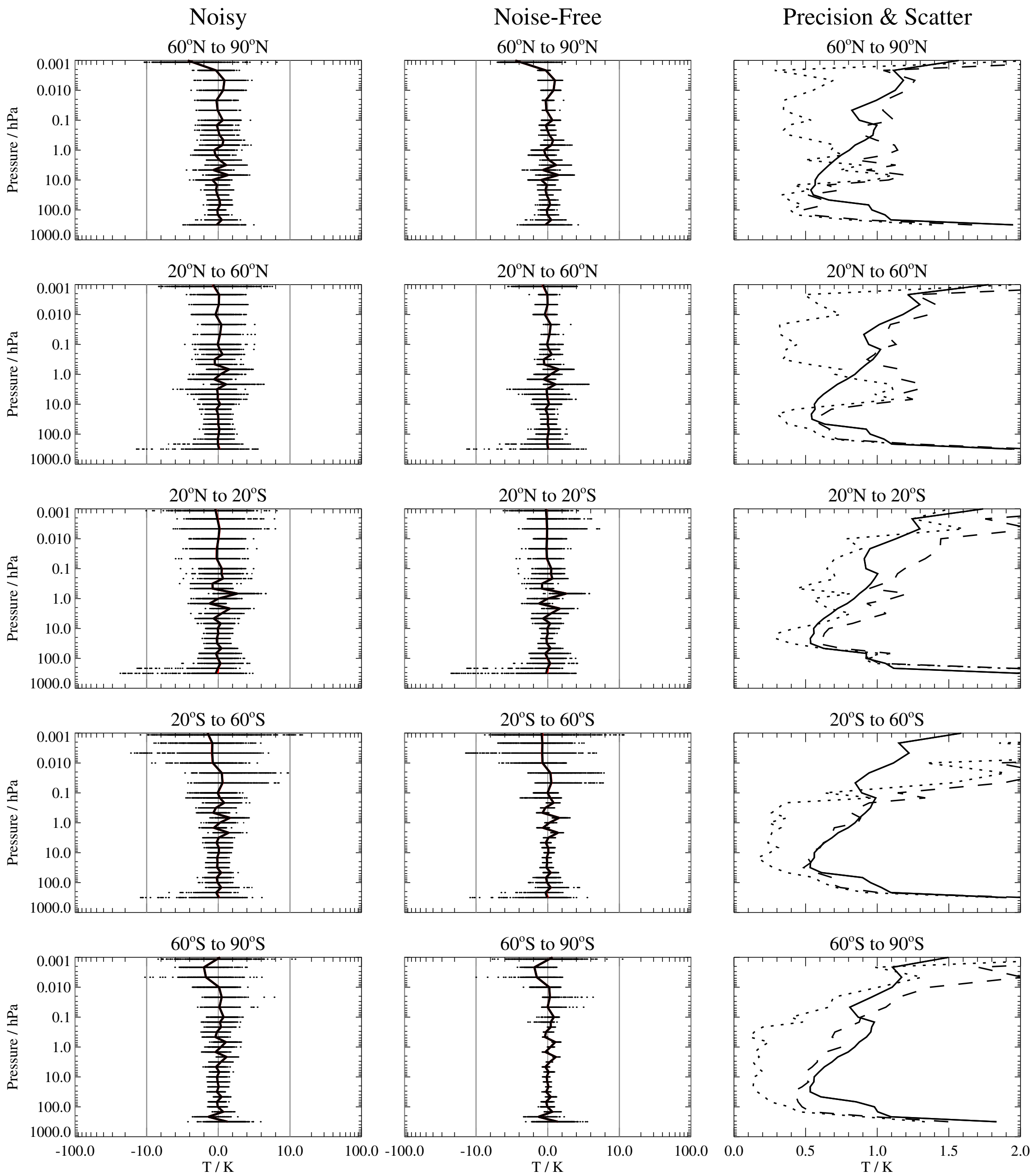

Figure 3.47: A summary of the v1.5 data quality for Temperature for the `1996d051` test dataset. Each row of panels represents a broad latitude bin. The first two columns show the differences between the retrieved Temperature and the true Temperature as a function of pressure, for the noisy and noise-free case, along with a solid line that shows the median bias. The median bias of the `Status=0` profiles (i.e., those not significantly affected by clouds) is shown in red. The final column shows the mean estimated precision of Temperature (solid line), and the rms scatter about the mean bias in the noisy (dashed line) and noise-free (dotted line) cases. Some of the plots in this figure use a mixed logarithmic/linear x-axis. The scale is linear in the region around zero bias and logarithmic beyond. In the logarithmic region decades are delimited with gray lines.

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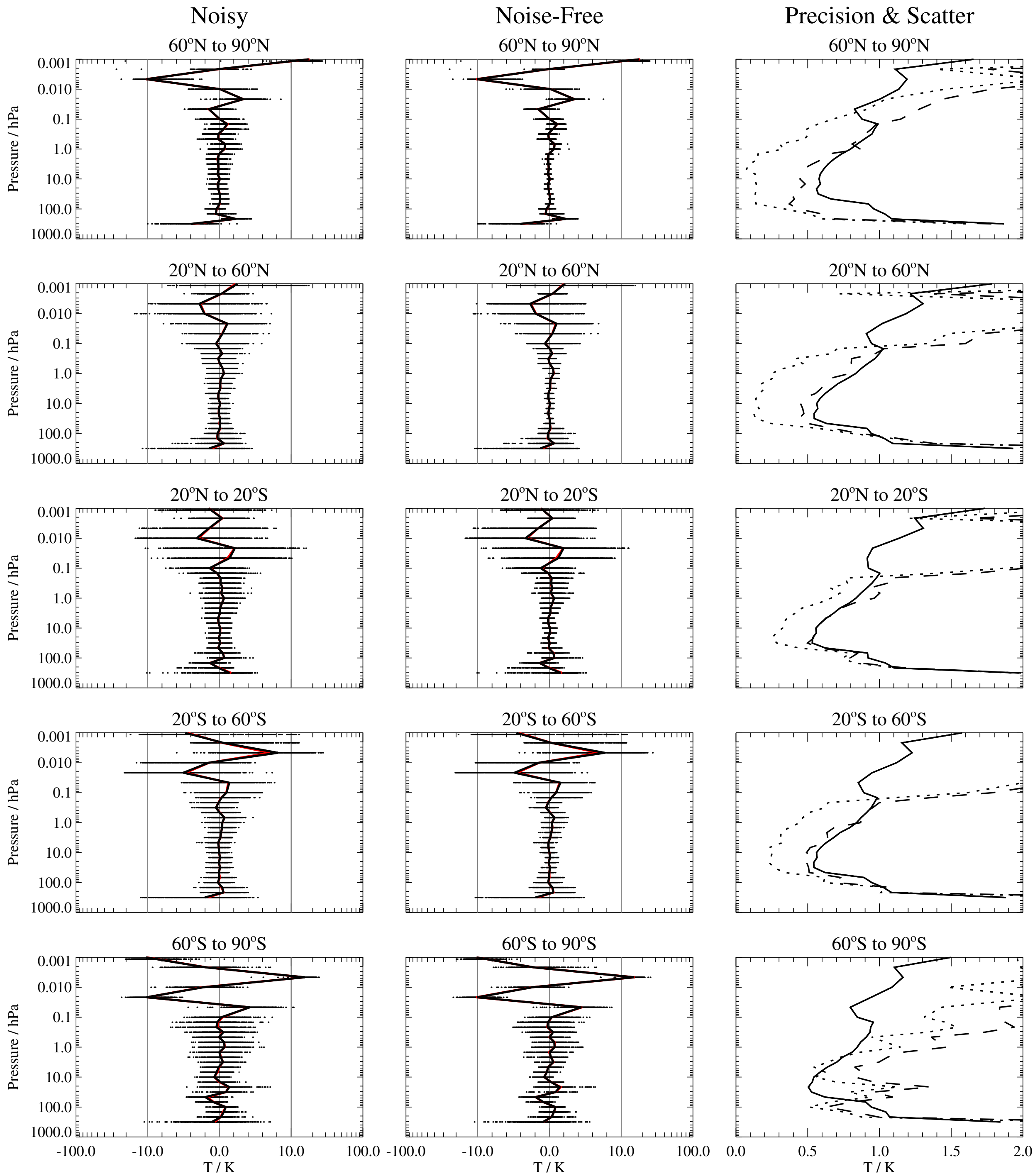

Figure 3.48: A summary of v1.5 data quality for Temperature as figure 3.47 for the `2000d276` test data set.

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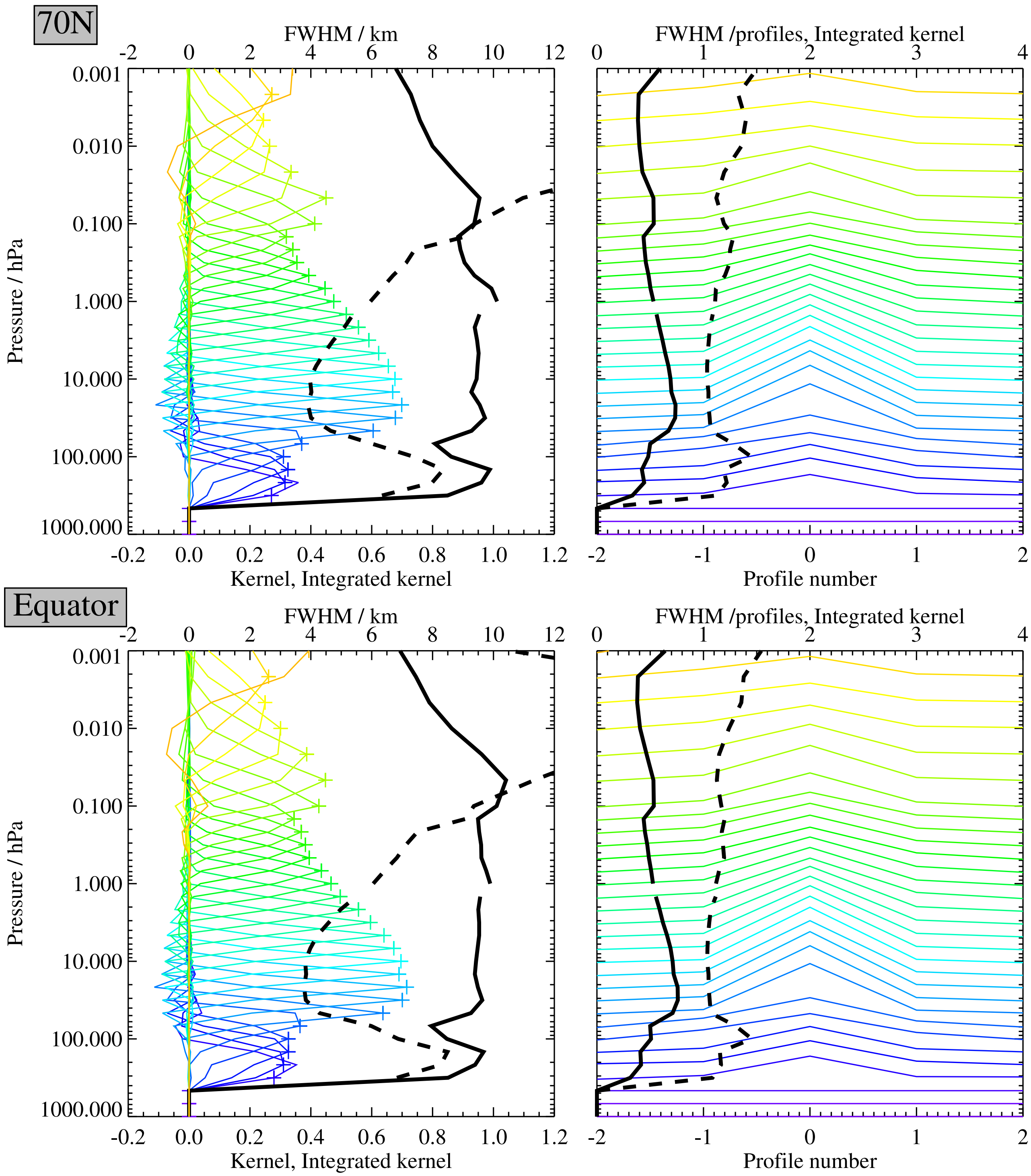

Figure 3.49: The left hand plots show the vertical averaging kernel for Temperature for the `1996d051` test data set. The colored lines denote the averaging kernels for individual retrieved surfaces (denoted with the matching color + symbols). The thick solid black line shows the integrated area under each colored line. The thick dashed black line denotes the vertical resolution (full width at half maximum) approximately scaled into kilometers. The right hand plots show the horizontal averaging kernels in a similar manner, where the profiles are spaced at 1.5° great circle angle (approximately 165 km).

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Data screening

Pressure range (316 – 0.001 hPa): Values outside this range are not suitable for scientific study.

Estimated Precision: Values at altitudes where the estimated precision is flagged negative should not be used, as they are strongly affected by the *a priori* (see section 1.3).

Status flag: Any profile for which `Status` is an odd number should not be used (see section 1.4).

Quality flag: Profiles with a value of the `Quality` field (see section 1.4) less than 1.0 should not be used. This flag is an indication of poor radiance fits (large χ^2) indicating that the radiances are not consistent with retrieved values even for reasonable-looking profiles. Less than 1% of Temperature profiles are discarded by this screening.

Artifacts

- There appears to be a 1 – 2 K warm bias in the stratosphere.
- The 10 hPa level shows a 2 – 4 K warm bias.
- There are vertical oscillations in the stratosphere and upper troposphere.

Priorities for future data version(s)

- Reduce vertical oscillations in retrievals.
- Improve vertical resolution in the troposphere and lowest stratosphere to ∼4 km by including information from more MLS bands than used to form the v1.5 standard product.
- Extend retrieval further into the troposphere.

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