

Validation of the Aura Microwave Limb Sounder stratospheric water vapor and nitrous oxide measurements

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Abstract. The quality of the version 2.2 (v2.2) stratospheric water vapor and nitrous oxide measurements from the Microwave Limb Sounder (MLS) on the Earth Observing System (EOS) Aura satellite is assessed. The impacts of the various sources of systematic error are estimated by a comprehensive set of retrieval simulations. Comparisons with correlative datasets from ground-based, balloon and satellite platforms operating in the uv/visible, infrared and microwave regions of the spectrum are performed. The stratospheric and mesospheric v2.2 H₂O data have been improved over v1.5 by providing higher vertical resolution in the lower stratosphere and better precision above the stratopause. The single-profile precision is $\sim 0.2\text{--}0.3$ ppmv (4–9%) and the vertical resolution is $\sim 3\text{--}4$ km in the stratosphere. The precision and vertical resolution become worse with increasing height above the stratopause. Over the pressure range 0.1–0.01 hPa the precision degrades from 0.4–1.1 ppmv (6–34%) and the vertical resolution degrades to $\sim 12\text{--}16$ km. The accuracy is estimated to be 0.2–0.5 ppmv (4–11%) for the pressure range 68–0.01 hPa. The scientifically useful range of the H₂O data is from 316–0.002 hPa. Substantial improvement has been achieved in the v2.2 N₂O data over v1.5 by reducing a significant low bias in the stratosphere and eliminating unrealistically high biased mixing ratios in the polar regions. The single-profile precision is $\sim 13\text{--}25$ ppbv (7–38%), the vertical resolution is $\sim 4\text{--}6$ km and the accuracy is estimated to be 3–70 ppbv (9–25%) for the pressure range 100–4.6 hPa. The scientifically useful range of the N₂O data is from 100–1 hPa.

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1. Introduction

Global measurements from spaceborne instruments over the last 30 years have provided important information on the middle atmosphere distributions of water vapor and nitrous oxide. In this paper we assess the quality of the daily global three-dimensional stratospheric water vapor and nitrous oxide version 2.2 data products from the Microwave Limb Sounder on the Earth Observing System Aura satellite launched in July 2004.

Water vapor is a highly variable atmospheric trace gas species and the dominant greenhouse gas. It plays a major role in all fundamental atmospheric processes involving radiation, chemistry, microphysics and dynamics on a vast range of characteristic spatio-temporal scales [Kley *et al.*, 2000]. Water vapor enters the middle atmosphere from the troposphere, through the tropical transition layer (TTL), where it undergoes a “freeze-drying” process which renders the stratosphere extremely dry. The photochemical stability of water vapor allows it to be used as a stratospheric tracer, however, above ~ 70 km the effects of photolysis reduces the lifetime to less than 10 days.

Nitrous oxide is produced almost entirely in the Earth’s biosphere by natural biological activity and agricultural processes. The surface abundance of this efficient greenhouse gas has increased from ~ 270 ppbv in pre-industrial times to ~ 319 ppbv in 2005 [WMO, 2006]. It is a well-mixed gas in the troposphere and displays a rapidly declining abundance with height in the stratosphere where it is destroyed mainly by photodissociation and also by reaction with excited oxygen forming the major source of reactive nitrogen oxides (NO_x) in the stratosphere. Since the photochemical lifetime of nitrous oxide ranges from 100 years at 20 km to a few months at 40 km and is longer than dynamical timescales, it an excellent tracer of transport processes throughout the stratosphere.

NASA’s Earth Observing System (EOS) Aura satellite, launched on July 15, 2004, is operated in a 98° inclination Sun-synchronous Earth orbit at an altitude of 705 km with a 1:45 P.M. ascending-node time. The Microwave Limb Sounder (MLS) [Waters *et al.*, 2006] is one of four instruments on board the Aura platform which has the main mission objective of studying ozone, air quality and climate [Schoeberl *et al.*, 2006]. MLS detects the thermal microwave emission from the Earth’s limb and retrieves vertical profiles of atmospheric temperature and composition in the vertical range 8–90 km [Livesey *et al.*, 2006]. Here we present the validation of the second public release of the Aura MLS stratospheric (and mesospheric) water vapor (H₂O) and nitrous oxide (N₂O) datasets, designated version 2.2 (v2.2). The v2.2 upper troposphere and lower strato-

sphere H₂O retrievals for pressures >68 hPa and comparisons against measurements by hygrometers for pressures >10 hPa are discussed separately in a companion paper [Read *et al.*, 2007].

The validation of the v2.2 MLS H₂O and N₂O retrievals involves assessing the data quality from the retrieval diagnostics and sensitivity studies, determining the precision and accuracy in conjunction with independent correlative measurements and providing data users with appropriate guidance on the use of the data for scientific studies. In Section 2 we describe the Aura MLS measurement characteristics related to the retrieval of H₂O and N₂O, recommend a data quality control procedure, discuss the precision and resolution of the retrieved products and present the results of investigations into the instrument and forward modeling systematic errors. Comparisons with correlative measurements are presented in Section 3 and the summary and conclusions are given in Section 4.

2. Aura MLS measurement characteristics

2.1. Overview

The Aura Microwave Limb Sounder [Waters, 1993; Waters *et al.*, 2006], an advanced successor to the MLS instrument on the Upper Atmosphere Research Satellite (UARS), is a limb sounding instrument which measures thermal emission at millimeter and sub-millimeter wavelengths using seven radiometers to cover five broad spectral regions. The radiometric and spectral performance of the MLS instrument is covered in detail by Jarnot *et al.* [2006] for the GHz radiometers and by Pickett [2006] for the THz radiometer. The standard H₂O and N₂O products are retrieved from the radiances measured by the radiometers centered near 190 GHz (R2), and 640 GHz (R4), respectively.

The MLS line-of-sight is in the forward direction of the Aura spacecraft flight track. The Earth’s limb is scanned from the surface to 90 km every 26.6 s giving 240 scans per orbit spaced at 1.5° intervals (165 km) with a total of ~ 3500 vertical profiles per day and a nearly global latitude coverage from 82°S–82°N. The viewing geometry of the MLS instrument allows the innovative use of a 2-dimensional approach to the retrieval problem since the limb observations from successive scans overlap significantly which means that effects of line-of-sight gradients can be taken into account [Livesey and Read, 2000].

At the time of writing (March 2007) reprocessing of the MLS data with the v2.2 algorithms is in progress and priority has been given initially to a set of days for which correlative measurements exist. Although fewer than 100 days covering all seasons have been reprocessed so far with v2.2,

these form a sufficient data record for a detailed investigation of the MLS data quality.

2.2. Guide to the appropriate use of the data

The MLS Level 2 Geophysical Product (L2GP) data consist of vertical profiles of the retrieved volume mixing ratios and their corresponding estimated precisions. The L2GP data are distributed in daily HDF-EOS version 5 swath format files [Livesey *et al.*, 2007]. The sign of the precision data field is used to flag the influence of the a priori information on the retrieved data. It is recommended that only data points with positive precision values be used, since negative precision values indicate that the a priori contributes significantly to the retrieval.

Version 2.2 has three quality metrics available to enable screening the data to remove profiles unsuitable for scientific studies. The ‘Status’ field (see Table 1) is a 32-bit integer in which the individual bits are set as necessary to indicate both instrumental and retrieval problems e.g. instrument anomalies, potential effects of clouds, error conditions that occurred during the data processing. Any profile for which ‘Status’ is an odd number should not be used in scientific studies. Nonzero but even values of ‘Status’ indicate that the profile has been marked as questionable, typically because the measurements may have been affected by the presence of thick clouds. Clouds generally do not have a significant impact (outside the noise) on the stratospheric H₂O and N₂O profiles and there is no apparent need to discard data points based on where ‘Status’ values indicate the existence/influence of clouds.

The ‘Quality’ field is a floating-point number which represents how well the calculated radiances from the retrieved data were fit to the observed radiances with small values of ‘Quality’ indicating a poor fit. We recommend only accepting profiles with ‘Quality’ values greater than 0.9 for H₂O and 0.5 for N₂O. These thresholds typically exclude 1% of the profiles on a typical day.

The ‘Convergence’ field (introduced in the v2.2 processing) is a floating-point number which represents how close the goodness-of-fit value (χ^2) in the final retrieval step came to the predicted χ^2 based on a linear extrapolation. Generally, large values of ‘Convergence’ indicate that satisfactory convergence was not achieved within the constraint of the maximum number of iterations allowed for the retrieval. It has not been found necessary to screen the H₂O profiles based on ‘Convergence’. There are, however, signs of poor convergence in some of the N₂O retrievals, resulting in sets of consecutive profiles that are temporally “smooth” at some levels. Data screening using the convergence field is recommended to remove these data points, therefore we recommend only accepting N₂O profiles with ‘Convergence’

values less than 1.55. This threshold typically excludes less than 5% of the profiles on a typical day.

2.3. Signatures of H₂O and N₂O in the MLS radiances

Sample radiance spectra for a representative day of Aura MLS observations are shown in Figures 1 and 2 for the H₂O and N₂O retrieval, respectively. Further details concerning the MLS spectral bands and target molecules are given by Waters *et al.* [2006] and Read *et al.* [2006].

H₂O The strong H₂O line at 183.31 GHz dominates the spectrum in Figure 1. There is only just visible contamination from N₂O line emission in the channels near 201.0 GHz in the upper sideband of band 2. These channels are not included in the retrieval because they overlap with band 3 which is centered on the N₂O line. The residuals indicate acceptably good fits of the forward model radiances to the observed radiances of $\sim 2\%$ for band 2 and of $\sim 5\%$ for band 23.

N₂O In addition to the N₂O line at 652.83 GHz in the upper sideband, strong spectral features are present in the spectrum in Figure 2 at both sides of band 12 from ozone emission lines in the channels near 633.4 GHz (O₃) in the lower sideband, and near 652.3 GHz (O₃(ν_2)) and 653.5 GHz (O₃(ν_2)) in the upper sideband. The channels with strong contaminating lines are not included in the retrieval. A small spectral feature is seen at the higher altitudes from contaminating species near 632.95 GHz (HNO₃ and O₃($\nu_{1,3}$)) in the lower sideband, and near 652.85 GHz (O¹⁸OO). The residuals indicate acceptably good fits of the forward model radiances to the observed radiances of $\sim 1\%$ for band 12.

2.4. Retrieval Method

The production of geophysical data (Level 2 data) from the calibrated observations of atmospheric limb radiances (Level 1 data) involves the Level 2 retrieval algorithms [Livesey *et al.*, 2006]. These employ an optimal estimation method [Rodgers, 1976, 2000] applied to the problem of a nonlinear weighted least squares minimization of a cost function involving the fit to the observed Level 1 radiance signals with regularization provided by a priori constraints. The MLS forward model [Read *et al.*, 2006; Schwartz *et al.*, 2006] takes into account the physics of the radiative transfer process and instrument specific parameters to calculate radiance estimates given a particular atmospheric state. The Level-2 processor invokes an inverse model that uses the forward model and a priori constraints in an iterative scheme, starting from an initial guess atmospheric state, to determine the optimal atmospheric state.

The MLS Level 2 processor is implemented as a series of retrieval phases. In the “Core” phase the standard product re-

retrievals of temperature/pressure [Schwartz *et al.*, 2007] and upper tropospheric humidity [Read *et al.*, 2007] are carried out and cloud detection is performed [Wu *et al.*, 2007]. This phase is then followed by the “Core+Rn” phases (n is the radiometer number) where the atmospheric species specific to the particular radiometer spectral region are retrieved. In each retrieval phase the Level 2 processor operates in parallel on ~ 350 data ‘chunks’ created by sub-dividing the Level 1 radiance scans into contiguous measurements in a 15° span of great circle angle (typically about 10 vertical profiles); retrievals are performed for each of these chunks independently and then joined together to produce the set of retrievals for a day.

H₂O The standard product for H₂O in v2.2 is retrieved from the limb emission measurements at 183.31 GHz in the “Core+R2” phase from the R2 190-GHz radiometer band 2 (25-channel filter-bank spectrometer) and band 23 (129-channel digital autocorrelator (DAC) spectrometer) which uses limb tangent heights with an optical depth cut-off of 0.4. Contaminating emission is present from O₃ (and excited states/isotopologues), HNO₃ and N₂O. These species are also retrieved simultaneously from other bands of the R2 radiometer, however, the N₂O retrieval from the “Core+R2” phase is currently considered a diagnostic product only and is not considered further here. The temperature and pressure data for this phase are constrained to the values retrieved from the “Core” phase [Schwartz *et al.*, 2007]. The H₂O profiles are retrieved on a pressure grid consisting of 12 levels per decade (spacing ~ 1.25 km) reducing to six levels per decade for pressures < 22 hPa and three levels per decade for pressures < 0.1 hPa. Because of the large variation in H₂O mixing ratio, the retrieval assumes that $\log(\text{mixing})$ ratio, and not mixing ratio itself, varies with \log -pressure. The recommended pressure range for single profiles for scientific studies is 316–0.002 hPa. Further details of the retrieval for this phase relevant to the upper troposphere are presented by Read *et al.* [2007].

N₂O The standard product for N₂O in v2.2 is retrieved from the limb emission measurements at 652.83 GHz in the “Core+R4B” phase from the R4 640-GHz radiometer band 12 (25-channel filter-bank spectrometer). Contaminating emission is present from O₃ (and excited states/isotopologues), HNO₃, H₂O and SO₂. The SO₂ is retrieved simultaneously, but the remaining contaminant species are constrained to the values obtained from previous retrieval phases. A simultaneous temperature/pressure retrieval is also performed in this phase using the O₂ bands in the the R1 (118-GHz) radiometer. The N₂O profiles are retrieved on a pressure grid consisting of six levels per decade (spacing ~ 2.5 km) reducing to three levels per decade for pressures < 0.1 hPa. The recommended pressure range for single profiles for scientific

studies is 100–1 hPa.

2.4.1. Data artifacts

H₂O The correlative measurement comparisons in Section 3 show a fine-scale oscillation in the v2.2 H₂O retrievals, whereby the mixing ratio at the 31.6 hPa (26.1 hPa) level is persistently low (high) by ≤ 0.4 ppmv (8%). Distributions of the differences in the H₂O values between these pressure levels (not shown) as a function of latitude and time indicates that larger amplitude oscillations can occur in the polar vortices and occasionally be reversed in sign. Rather than attempting a correction using fixed additive offsets, we suggest replacing the values at the 31.6 hPa and 26.1 hPa levels with their average for investigations that are impacted by the presence of the oscillation using the following algorithm: if $v_{31.6} < v_{38.3}$ and $v_{31.6} < v_{26.1}$ and $v_{21.5} < v_{26.1}$ then $v_{31.6} = v_{26.1} = (v_{31.6} + v_{26.1})/2$, where v_p is the volume mixing ratio at the pressure level p in hPa.

Note that the H₂O retrieval uses $\log(\text{mixing ratio})$ and the allowed H₂O values are constrained to be positive by applying a low bound of 0.1 ppmv.

N₂O The allowed N₂O values are restricted in the retrieval to a low bound of -40 ppbv (approximately three times the retrieval noise level in the recommended pressure range) in order to prevent a problem occurring in the minimization search process. The low bound is applied at all levels, but it is only evident in the data for pressures ≤ 0.1 hPa, where the vertical smoothing is relaxed and the retrieval noise becomes comparable to the magnitude of the low bound value. Statistical averaging of the N₂O data (zonal means or longer time periods) cannot be applied successfully for pressures ≤ 0.1 hPa as the result will be to produce estimates with a positive bias. The N₂O values on the 147 hPa pressure level have a large a priori influence and practically all precisions are flagged negative at this level.

2.5. Precision and resolution

The formal retrieval precision estimates are the square root of the diagonal elements (variances) of the solution covariance matrix and are to be interpreted as the theoretical $1-\sigma$ uncertainties in the retrieved values. In the case of significant contribution of the a priori to the retrieved data the sign of the corresponding precision estimate is set negative by the Level 2 processor. This is effected for each pressure level where the formal precision value is greater than 50% of the a priori precision.

A simple method of validating the formal retrieval precision estimates is to compare retrieved profile pairs at the intersections of ascending/descending orbits. The mean difference of the profile pairs can be useful for indicating biases in the measurement system and the observed scatter (i.e.

standard deviation (SD)) about the mean differences should be ideally $\sqrt{2}$ times the precision on the individual measurements. In practice, systematic biases and increased scatter may arise from atmospheric variability (e.g. diurnal changes in concentrations, tidal effects) or residual instrument orbital effects occurring on the timescale (12 hours) of the repeated measurements. The observed scatter then provides an upper limit for the precision estimates provided that the a priori has a negligible influence on the retrieval. In Figures 3 and 4 we show the results of this analysis for a large number of ascending/descending profile matches in the latitude range 50°S–50°N, where the SD values have been scaled by $1/\sqrt{2}$. Hence, in this case, the observed SD represents the statistical repeatability of the MLS measurements and the expected SD represents the theoretical 1- σ precision for a single profile.

For H₂O the systematic bias in Figure 3 is small but becomes more pronounced in the mesosphere where tides may have an effect. The observed and expected SD are in reasonable agreement from 100–0.1 hPa. For pressures <0.1 hPa the observed SD is smaller than the expected SD indicating an increased influence of the a priori. For pressures >100 hPa atmospheric variability increases the observed SD beyond that expected from the precision estimates alone. The estimated precision on a single retrieved profile is ~ 0.2 – 0.3 ppmv (4–9%) in the stratosphere. For N₂O the systematic bias in Figure 4 is small, but more pronounced at the bottom and top of the retrieval range, which is also where the observed SD is smaller than the expected SD indicating an increased influence of the a priori. The estimated precision on a single retrieved profile is ~ 13 – 25 ppbv (7–38%) for pressures 100–4.6 hPa.

The horizontal and vertical grids used in the Level 2 processing do not represent the actual spatial resolution of retrieved species as the second-order Tikhonov regularization [Rodgers, 2000] applied to stabilize the retrieval system degrades the intrinsic resolution [Livesey et al., 2006]. The spatial resolution is obtained from examination of the averaging kernel matrices shown in Figures 5 and 6. For H₂O the vertical (along-track horizontal) resolution is better than 4 km (410 km) below the stratopause, but becomes worse than 10 km in the mesosphere. The across-track horizontal resolution of 7 km is set by the 190-GHz antenna pattern [Cofield and Stek, 2006]. For N₂O the vertical (along-track horizontal) resolution is 4–5 km (300–600 km) over most of the useful range of the retrievals and the across-track horizontal resolution of 3 km is set by the 640-GHz antenna pattern [Cofield and Stek, 2006].

2.6. Quantification of systematic errors

A major component of the validation of MLS data is the quantification of the various sources of systematic uncer-

tainty. Systematic uncertainties arise from instrumental issues (e.g. radiometric calibration, field of view characterization), uncertainties in spectroscopic databases, and approximations in the retrieval formulation and implementation. This section summarizes the relevant results of a comprehensive quantification of these uncertainties that was performed for all MLS products. More information on this assessment is given in Appendix A of Read et al. [2007].

The impact on MLS measurements of radiance (or pointing where appropriate) of each identified source of systematic uncertainty has been quantified and modeled. These modeled impacts correspond to either 2- σ estimates of uncertainties in the relevant parameters, or an estimate of their maximum reasonable errors based on instrument knowledge and/or design requirements. The effect of these perturbations on retrieved MLS products has been quantified for each source of uncertainty by one of two methods.

In the first method, sets of modeled errors corresponding to the possible magnitude of each uncertainty have been applied to simulated MLS cloud-free radiances, based on a model atmosphere, for a whole day of MLS observations. These sets of perturbed radiances have then been run through the routine v2.2 MLS data processing algorithms, and the differences between these runs and the results of the ‘unperturbed’ run have been used to quantify the systematic uncertainty in each case. The impact of the perturbations varies from product to product and among uncertainty sources. Although the term ‘systematic uncertainty’ is often associated with consistent additive and/or multiplicative biases, many sources of ‘systematic’ uncertainty in the MLS measurement system give rise to additional scatter in the products. For example, although an error in the ozone spectroscopy is a bias on the fundamental parameter, it has an effect on the retrievals of species with weaker signals that is dependent on the amount and morphology of atmospheric ozone. The extent to which such terms can be expected to average down is estimated to first order by these ‘full up studies’ through their separate consideration of the bias and scatter each source of uncertainty introduces into the data. The difference between the retrieved product in the unperturbed run and the original ‘truth’ model atmosphere is taken as a measure of the uncertainties due to retrieval formulation and numerics. Sensitivity of the retrieved mixing ratio to the a priori mean value has been assessed by performing a retrieval of the unperturbed radiances after adjusting the standard MLS a priori by a factor of 1.5.

In the second method, the potential impact of some remaining (typically small) systematic uncertainties has been quantified through calculations based on simplified models of the MLS measurement system [Read et al., 2007]. Unlike the ‘full up studies’, these calculations only provide es-

timates of the percentage bias error introduced by the source in question; this approach is unable to quantify additional scatter for these minor sources of uncertainty.

Figures 7 and 8 summarize the results of the uncertainty characterization for the MLS v2.2 H₂O and N₂O measurements, respectively. The colored lines show the magnitudes of expected biases and scatter that the various sources of uncertainty may introduce into the data, and should be interpreted as 2- σ estimates of their probable magnitude.

Although the MLS observations are unaffected by thin cirrus clouds or stratospheric aerosols, thick clouds associated with deep convection can have an impact on the MLS radiances. The MLS Level 2 data processing algorithms discard radiances identified (through comparison with predictions from a clear-sky model) as being strongly affected by clouds [Livesey *et al.*, 2006; Wu *et al.*, 2007]. The contribution of cloud effects to the systematic uncertainty, both from the presence of clouds not thick enough to be screened out by the cloud filtering and from the loss of information through omission of cloud-impacted radiances, has been quantified by adding scattering from a representative cloud field to the simulated radiances and comparing retrievals based on these radiances to the unperturbed results. The cloud-induced effects are estimated by considering only the cloudy profiles (as defined by the known amount of cloud in the ‘truth’ field).

H₂O In Figure 7 the largest potential source of systematic bias for pressures > 0.2 hPa is $\sim 3\%$ from the pointing uncertainty (red line) arising from the field of view pointing offsets between the radiometers used in the “Core” and “Core+R2” retrievals and the O₂ line width uncertainty. The dominant bias for pressures < 0.2 hPa originates from a source termed ‘gain compression’, whereby departures from a linear response within the signal chains (cyan line) introduce a spectral signature in the calibrated MLS radiances. This bias is in the range 10–25% for pressures < 0.01 hPa and also has a worst-case effect of $\sim 8\%$ in the lower stratosphere at the 31.6–26.1 hPa levels. Compensating for gain compression in the Level 1 processing is under investigation, but has not been carried out for the v2.2 retrievals. The bias arising from the a priori (gray line) is seen to be $\sim 8\%$ in the range 32–4.6 hPa and 10–20% in the range 0.01–0.002 hPa, but is <2% outside these regions. The uncertainty on the H₂O spectral line width (green line) is responsible for a bias of $\sim 3\%$. Cloud-induced effects (black line) lead to negligible bias in the H₂O retrieval for pressures ≤ 68 hPa. Other potential sources of uncertainty are found to contribute negligibly to the bias. The aggregate scatter is comparable to the bias.

N₂O In Figure 8 the largest potential source of systematic bias (≤ 30 ppbv) over most of the profile range arises

from the radiometric/spectroscopic contributions (cyan line) of gain compression, sideband fraction, and standing waves. The spectroscopic uncertainty (green) is composed of a 20 ppbv bias in the lower stratosphere from the N₂O spectral line width and a worst-case bias of 15 ppbv at 100 hPa from the N₂ continuum. The O₃ contaminant species uncertainty (blue line) contributes a bias of up to 6 ppbv. The pointing uncertainty (red line) is <5 ppbv for pressures ≤ 46 hPa rising to 27 ppbv at 100 hPa and arises from the field of view pointing offsets between the radiometers used in this retrieval (R1 and R4) and the O₂ line width uncertainty. The bias arising from the a priori (gray line) gives the largest contribution of 55 ppbv at 100 hPa. Cloud-induced effects (black line) lead to biases in the N₂O retrieval of <1 ppbv except at 100 hPa, where the bias is 5 ppbv. Other potential sources of uncertainty are found to contribute negligibly to the bias. The aggregate scatter is negligible compared to the bias.

2.7. Comparison of the v2.2 and v1.5 MLS datasets for H₂O and N₂O

The first public release of the MLS dataset was version 1.5 (v1.5) and it has been used to operationally process all data from launch to March 2007. Early validation of the v1.5 dataset is discussed by Froidevaux *et al.* [2006]. Since the v1.5 H₂O and N₂O data have already been used in scientific studies [e.g. Jimenez *et al.*, 2006; Manney *et al.*, 2006], we compare these datasets and discuss their differences in this section.

H₂O In addition to the v2.2 H₂O product being produced on a higher vertical resolution basis grid than for v1.5, there are a number of other important changes to the retrieval. The temperature and pressure retrieval has been eliminated from the “Core+R2” phase and the optical depth cut-off for band 2 has been increased from 0.2 to 0.4. The same cut-off has been applied to band 23, which is a narrow band (10 MHz) digital autocorrelator spectrometer included the v2.2 retrieval to improve the sensitivity in the mesosphere by resolving the narrow-line Doppler-broadened emission. The spectroscopy for H₂O has been updated by increasing the H₂O line strength by 0.7% and increasing the line width by 4% (see Read *et al.* [2007] for details). Figure 9 shows the global mean v1.5 and v2.2 H₂O profiles, precisions and mean differences averaged over 92 days of data. The v2.2 H₂O data product is similar to v1.5 for pressures > 0.1 hPa, except that near the stratopause v2.2 has values up to 0.5 ppmv larger and there is an oscillation present at the 31.6–26.1 hPa levels which is also seen in the comparisons to correlative data in Section 3. The amplitude of oscillations at other levels reported in the v1.5 data by Froidevaux *et al.* [2006] has been reduced in v2.2.

The precisions are significantly better in v2.2 especially in the mesosphere, where the addition of band 23 contributes to the retrieval as discussed above. For pressures < 0.1 hPa the majority of the v1.5 precision data were set to negative values indicating a larger a priori influence than in v2.2.

N₂O The v2.2 N₂O product uses a more accurate forward model for the calculation of radiances in band 12 in the lower stratosphere (> 10 hPa) than for v1.5. A linearized forward model was used for v1.5 based on pre-computed radiances and derivatives for monthly climatological atmospheric states (binned in pressure and latitude). The accuracy is limited by the extent of the departure of the true state from the a priori state (linearization point) and is generally poorer in the winter polar vortexes. Figure 10 shows the global mean v1.5 and v2.2 N₂O profiles, precisions, and mean differences averaged over 92 days of data. The v2.2 N₂O product is systematically 5–15% larger than v1.5 in the region 46–2.2 hPa, but at 68 hPa and 100 hPa it is 6% and 15% smaller, respectively. The v2.2 N₂O product has slightly better precision values than in v1.5. In the lower stratosphere (≥ 68 hPa) polar vortex and near vortex regions the v1.5 linear forward model approximation for the N₂O retrieval occasionally led to unrealistically high biases which can be seen in Figure 11. An off-line post-processing data mask was made available for the v1.5 N₂O data [Livesey *et al.*, 2005] to screen out the biased data points (not applied in the figure shown here). However, as the comparison in Figure 11 shows, these high biases have been eliminated in the v2.2 data through the use of a more accurate forward model.

3. Correlative data comparisons

We assess the accuracy of the Aura MLS v2.2 H₂O and N₂O measurements using correlative data from spaceborne, ground-based and balloon platforms. All the comparisons have been performed using simple temporal and geometric spatial coincidence matching of the MLS profiles with the correlative instrument. In order to calculate differences, the correlative profiles were first linearly interpolated in log-pressure to the fixed MLS retrieval pressure grid used for a particular species. Individual profile comparisons for the balloon data are presented on their native pressure surfaces. Since in most cases the vertical resolution of the correlative measurements is comparable to that of MLS, no further processing involving averaging kernel smoothing has been applied, except as described in Section 3.2 for the ground-based data. For the spaceborne and ground-based data the statistics presented are (1) the ensemble global mean species profiles of the collocated matches for both instruments; (2) the mean percentage and absolute species differences be-

tween the two instruments (MLS–‘correlative’); (3) the observed standard deviations (SD) about the mean differences; (4) the expected standard deviations calculated from the root sum square of the precisions on the species measurements from the two instruments.

3.1. Spaceborne instruments

In this section we present contemporaneous measurement comparisons from a variety of solar occultation and limb-emission instruments operating in the uv/visible, infrared and microwave wavelength regions. The latitude and time sampling of the comparisons with each of the correlative instruments is shown in Figure 12.

3.1.1. ACE-FTS The Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) [Bernath *et al.*, 2005] was launched in August 2003 on the Canadian Space Agency SCISAT-1 satellite into a 74° inclination orbit and uses high resolution (0.02 cm⁻¹) infrared solar occultation in the spectral region 2.3–13.3 μm (750–4400 cm⁻¹) to measure atmospheric temperature and concentrations of more than 20 species, including H₂O and N₂O which are retrieved using selected micro-windows in the 953–2000 cm⁻¹ and 1121–2668 cm⁻¹ range, respectively. Nominally, fifteen sunrise and sunset profiles are obtained per day. The latitude coverage is 85°S – 85°N and the vertical range is from 5 km (or cloud top) to 150 km with a typical vertical resolution of 4 km with typical precisions of <5% for H₂O and <5% for N₂O. The version 2.2 ACE-FTS data are used here [Boone *et al.*, 2005].

Analyses in equivalent latitude/potential temperature coordinates comparing both H₂O and N₂O observed by ACE-FTS and MLS during several multi-day intervals (using v2.2 MLS data), and comparing the evolution over the entire 2004/2005 Arctic winter (using v1.5 MLS data), are shown in a companion paper by Manney *et al.* [2007]. These analyses show good overall agreement in the morphology and timing of observed features in the two datasets.

Figures 13 and 14 compare all coincident profiles obtained within $\pm 1^\circ$ in latitude, $\pm 8^\circ$ in longitude, and ± 12 hours from 121 days of ACE-FTS data.

H₂O Figure 13 shows very good agreement to better than $\pm 5\%$ for nearly the entire pressure range 68–0.004 hPa (apart from the 31.6–26.1 hPa levels). The observed and expected SD are in good agreement, with the observed SD becoming smaller than the expected SD for pressures < 0.1 hPa in the mesosphere; most likely indicating an increasing a priori influence on the MLS data since the precisions on the ACE-FTS data (not shown) do not change markedly. Very similar results were found when the analysis was repeated for the separate ACE-FTS sunrise/sunset events (not

shown).

N₂O Figure 14 shows very good agreement with ACE-FTS to better than $\pm 5\%$ for nearly the entire pressure range 100–1 hPa with a low bias (up to -5%) in MLS for pressures >32 hPa and a high bias (up to $+5\%$) at lower pressures. The latitudinal distribution of the mean differences is presented in Figure 15, where it is seen that MLS v2.2 N₂O is systematically lower at nearly all latitudes in the pressure range 100–32 hPa. This also shows the separate ACE-FTS sunrise/sunset events and in general the sunrise events show smaller biases (MLS–ACE-FTS) for the pressure levels 46–10 hPa than do the sunset events. The observed SD is smaller than the expected SD for pressures < 6.8 hPa.

3.1.2. HALOE The Halogen Occultation Experiment (HALOE) [Russell et al., 1993] was launched on the Upper Atmosphere Research Satellite (UARS) into a 57° inclination orbit in September 1991 and uses infrared solar occultation in four radiometer channels and four radiometer/gas-filter correlation channels in the spectral region 2.45–10.0 μm to measure atmospheric temperature, aerosols, and composition including H₂O in the 6.6 μm band. Nominally, fifteen sunrise and sunset profiles are obtained per day. The latitude coverage is 80°S – 80°N ; the vertical range is from 15–85 km with a vertical resolution of 2.3 km and typical precisions of ~ 1 – 15% in the stratosphere for H₂O. The version 19 (v19) HALOE dataset is used; this has been described by Harries et al. [1996] and in the SPARC water vapor report [Kley et al., 2000]. The HALOE data are pre-screened for cloud effects before distribution.

As discussed by McHugh et al. [2005], H₂O comparisons should be limited to pressures > 0.02 hPa because of the possible contamination of the HALOE H₂O data by polar mesospheric clouds (PMCs) at certain times of the year. Figure 16 compares all coincident profiles obtained within $\pm 1^\circ$ in latitude, $\pm 8^\circ$ in longitude, and ± 12 hours from 53 days of HALOE data. MLS H₂O is larger than HALOE by 2–10% in the pressure range 68–1.5 hPa (apart from the 31.6–26.1 hPa levels). For pressures ≤ 1 hPa the bias is in the range 10–15%. Very similar results were found when the analysis was repeated for the separate HALOE sunrise/sunset events (not shown). The HALOE H₂O data have been previously reported as having a 5% dry bias in the stratosphere [Kley et al., 2000] and this is consistent with the results of this comparison. The observed and expected SD are in good agreement in the pressure range 68–2.2 hPa, where the HALOE precisions (not shown) are comparable to those from MLS.

3.1.3. SAGE II The Stratospheric Aerosol and Gas Experiment II (SAGE II) [McCormick, 1987] was launched into a 57° inclination orbit in October 1984 on the Earth Radiation Budget Satellite (ERBS). SAGE II uses ultravi-

olet/visible solar occultation in seven channels from 380–1020 nm to measure aerosol extinction at four wavelengths and the concentrations of O₃, H₂O and NO₂. The latitude coverage is 70°S – 70°N and the vertical range is from cloud tops to 70 km with a resolution of ~ 0.5 km. Fifteen sunrise and sunset profiles are obtained per day, although since November 2000 SAGE II has been operated with a 50% duty cycle. The version 6.2 [Taha et al., 2004] H₂O data uses a modified spectral filter band pass with the selected filter position (centered at 945 nm) and width determined by an empirical minimization of the mean bias of SAGE II retrievals with respect to a 10-year (1992–2002) v19 HALOE climatology [Thomason et al., 2004]. The agreement with HALOE is within 10% in the altitude range 15–40 km. Typical precisions for H₂O are ~ 15 – 35% in the stratosphere. The SAGE II H₂O data were screened as recommended to remove data points with correspondingly high aerosol extinctions (1020 nm extinction $> 2 \times 10^{-4}$).

Figure 17 compares all coincident profiles obtained within $\pm 1^\circ$ in latitude, $\pm 8^\circ$ in longitude, and ± 12 hours from 87 days of SAGE II data. MLS H₂O is larger than SAGE II by 5–10% (apart from the 31.6–26.1 hPa levels) in the pressure range 68–4.6 hPa with the bias changing sign in the upper stratosphere above this range which is consistent with the validation results of Taha et al. [2004]. Similar results were found when the analysis was repeated for the separate SAGE II sunrise/sunset events (not shown). The observed SD is significantly smaller than the expected SD and is most likely due to a pessimistic estimate of the SAGE II precisions, which are reported by Chiou et al. [2004] to be overestimated by a factor of 2–3 in the lower stratosphere.

3.1.4. POAM III The Polar Ozone and Aerosol Measurement III (POAM III) [Lucke et al., 1999] was launched in March 1998 on the French Space Agency SPOT-4 satellite into a polar Sun-synchronous orbit and uses ultraviolet/visible solar occultation in nine spectral channels in the region 345–1018 nm to measure aerosol extinction at six wavelengths and the concentrations of O₃, H₂O and NO₂. The H₂O observations use differential channels (on-peak/off-peak) in the 940 nm band. Fourteen sunrise and sunset profiles are obtained per day. However, to extend the instrument lifetime, the nominal observing scheme was changed to alternate between sunrise and sunset observations after the first year of operation, giving an effective 50% duty cycle. The latitude coverage is 63° – 88° S (all spacecraft sunset observations, but corresponding to local sunrise from mid-April to mid-September else local sunset) and 55° – 71° N (all spacecraft sunrise observations, but corresponding to local sunset) and the vertical range is from cloud tops to 50 km with a vertical resolution of 1–1.5 km which degrades to 3 km at 40 km. Typical precisions for

H₂O are 5–7% in the stratosphere. The version 4 POAM III dataset is used here [Lumpe *et al.*, 2006] and the H₂O data were screened for sunspot errors and aerosol contamination.

Figure 18 compares all coincident profiles obtained within $\pm 1^\circ$ in latitude, $\pm 8^\circ$ in longitude, and ± 12 hours from 92 days of POAM III data. MLS H₂O is smaller than POAM III by 10% over most of the range 68–1 hPa (apart from the 31.6–26.1 hPa levels). In a repeat of the analysis for the separate POAM III spacecraft sunrise/sunset events (not shown), the sunset events were found to give a 5–10% larger negative bias (MLS–POAM III) than the sunrise. These results are consistent with the POAM III validation analysis of Lumpe *et al.* [2006] who report for the 12–35 km range a high bias of 5–10% for sunrise events and an additional $\sim 10\%$ greater bias for sunset. The observed and expected SD are in reasonable agreement for pressures > 10 hPa.

3.1.5. MIPAS The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) [Fischer and Oelhaf, 1996] was launched on the European Space Agency (ESA) Environmental Satellite (Envisat) in March 2002 into a 98.5° inclination orbit. MIPAS is a Fourier Transform Spectrometer detecting the limb emission in the infrared spectral region $685\text{--}2410\text{ cm}^{-1}$ ($4.15\text{--}14.6\text{ }\mu\text{m}$) with a spectral resolution of 0.025 cm^{-1} . MIPAS operations were suspended in March 2004 due to an interferometer mechanism anomaly and then were restarted in January 2005 with a degraded spectral resolution of 0.0625 cm^{-1} and modified duty-cycle and scan sequence to extend instrument life-time [Piccolo and Dudhia, 2007]. MIPAS observes temperature, aerosols and a large number of minor constituents including H₂O and N₂O. The horizontal along-track sampling interval of the MIPAS measurements taken in the nominal reduced-resolution mode is ~ 410 km, latitude coverage is $90^\circ\text{S--}90^\circ\text{N}$, and the vertical sampling is $\sim 1.5\text{--}4$ km with a vertical range 6–70 km. In addition to the ESA operational data products [Raspollini *et al.*, 2006], several institutions funded by the ENVISAT Calibration/Validation Program have developed off-line data processing capabilities for MIPAS. Here we show comparisons with off-line MIPAS H₂O and N₂O retrievals from algorithms developed at the University of Oxford (personal communication, A. Dudhia and C. Waymark, 2006). The MIPAS profiles were supplied with a cloud flag for data screening.

Figures 19 and 20 compare all coincident profiles obtained within $\pm 1^\circ$ in latitude, $\pm 4^\circ$ in longitude, and ± 12 hours for January 28, 2005.

H₂O MLS is smaller than MIPAS by $\sim 10\%$ in the pressure range 22–2.2 hPa, and there are positive biases of $\sim 20\%$ at 0.2 hPa and 25% at 46 hPa, but no significant bias in the pressure range 1.5–0.68 hPa. The observed and expected SD show good reasonable agreement in the pressure range 22–

0.68 hPa.

N₂O MLS and MIPAS agree to about $\pm 5\%$ in the pressure range 32–1 hPa. The 68–46 hPa pressure region shows a positive bias of $\sim 10\text{--}15\%$ and the 100 hPa level shows a negative bias of $\sim 10\%$. The observed and expected SD show good agreement in the pressure range 32–4.6 hPa.

3.1.6. Odin/SMR The Sub-Millimetre Radiometer (SMR) [Murtagh *et al.*, 2002] was launched on the Odin Satellite in February 2001 into a Sun-synchronous near polar 97.8° inclination orbit and uses sub-millimeter wave heterodyne spectroscopy to detect limb emission in the spectral region 486–581 GHz to measure atmospheric temperature and the concentrations of trace species including N₂O from retrievals at 502.296 GHz. The stratospheric measurement mode is time-shared with astronomy and other aeronomy modes and operates on one day out of three. The horizontal along-track sampling interval is ~ 600 km, the latitude coverage is $82.5^\circ\text{S--}82.5^\circ\text{N}$ and the vertical scan range is 7–70 km. Profiles of N₂O are retrieved in the range $\sim 12\text{--}60$ km with a vertical resolution of 1.5 km in the lower stratosphere which degrades with increasing altitude to ~ 3 km in the upper stratosphere [Urban *et al.*, 2005b, 2006]. The single-profile precision is in the range 10–30 ppbv. Operational Level 2 retrievals are produced by the Chalmers University of Technology (Göteborg, Sweden) and here we use the version 2.1 N₂O data which is similar to version 2.0 [Urban *et al.*, 2006]. The estimated systematic error is ≤ 12 ppbv above 20 km and in the range 12–35 ppbv below. An off-line reference processing system has been developed at the Observatoire Aquitain des Sciences de l'Univers (Floirac, France). The retrieval methodology and error characterization for the Chalmers version 1.2 data, and the differences between the French and Swedish data processing systems, are described in detail by Urban *et al.* [2005a]. Barret *et al.* [2006] compared the Bordeaux v222 reference version data to MLS 1.5 data, and Urban *et al.* [2006] describe the main differences between Chalmers v1.2, Bordeaux v222 and Chalmers v2.0 data and include a comparison with MIPAS off-line data. Only good quality SMR data points are included in these comparisons (i.e. assigned flag QUALITY = 0, and a measurement response for each retrieved mixing ratio larger than 0.75 to ensure that the information has been derived from the measurements, with negligible contribution from the a priori profile [Urban *et al.*, 2005b; Barret *et al.*, 2006]).

Figure 21 compares all coincident profiles obtained within $\pm 1^\circ$ in latitude, $\pm 4^\circ$ in longitude, and ± 12 hours from 49 days of SMR data. MLS N₂O is smaller than SMR by $\leq 5\%$ in the pressure range 68–4.6 hPa and 10% smaller at 100 hPa. The observed and expected SD show reasonable agreement.

3.2. Ground-based instruments

The Naval Research Laboratory (NRL) operates three Water Vapor Millimeter-wave Spectrometer (WVMS) [Nedoluha *et al.*, 1997] operates three instruments deployed at sites in the Network for the Detection of Atmospheric Composition Change (NDACC) which measure the emission from the 22 GHz H₂O transition. The data used here are daily averaged measurements from two NDACC sites: WVMS1 at the National Institute of Water and Atmospheres Research (NIWA), Lauder (45.0°S, 169.7°E) and WVMS3 at the Mauna Loa Observatory, Hawaii (19.5°N, 204.4°E). The vertical range is 40–80 km with a vertical resolution of 10–20 km. In this case, since the MLS and WVMS instruments have quite different vertical resolutions, an appropriate inter-comparison was achieved by first convolving the MLS retrievals with the WVMS averaging kernels using methods described by Rodgers and Connor [2003]. The time sampling of the comparisons with the WVMS instruments is shown in Figure 12.

Figures 22 and 23 compare all coincident profiles obtained within $\pm 1^\circ$ in latitude, $\pm 8^\circ$ in longitude, and ± 12 hours from 66 (58) days of Mauna Loa (Lauder) data. MLS H₂O and both WVMS sites agree to within $\pm 5\%$ for the pressure range 3.2–0.15 hPa, with a positive bias for pressures < 0.32 hPa increasing to $\sim 10\%$ at 0.046 hPa. Time-series comparisons of WVMS and v1.5 MLS H₂O by Nedoluha *et al.* [2007] show good agreement in the seasonal and the inter-annual variations.

3.3. Balloon-borne instruments

In this section we consider the data from in situ and remote sounding balloon-borne instruments obtained during two Aura validation campaigns at Ft. Sumner, NM (34.4°N, 104.2°W) in September, 2004 and September, 2005.

3.3.1. Observations of the Middle Stratosphere (OMS) Gondola The in situ measurements presented are from two instruments flown on the OMS gondola that provided measurements of N₂O. The vertical range is typically from the upper troposphere to 32 km.

The Lightweight Airborne Chromatograph Experiment (LACE) [Moore *et al.*, 2003] is a three-channel gas chromatograph which provides in situ profiles of various gases including N₂O. The precision is estimated to be 1–2% and the vertical resolution is 0.3 km. The Cryogenic Whole Air Sampler (CWAS) [Hurst *et al.*, 2002] collects in situ air samples in canisters which are analyzed for N₂O using electron-capture gas chromatography. The precision is estimated to be 1% and the vertical resolution is 0.3 km.

3.3.2. Balloon Observations of the Stratosphere (BOS) Gondola The remote sounding measurements presented

are from three instruments flown on the BOS gondola that provided measurements of H₂O and N₂O.

The Jet Propulsion Laboratory (JPL) MkIV instrument [Toon, 1991] is a Fourier Transform Infrared (FTIR) spectrometer operated in solar occultation mode that measures over the entire 650–5650 cm⁻¹ region with 0.01 cm⁻¹ resolution. The vertical range is 8–40 km with a vertical resolution of 2–3 km. The MkIV H₂O retrievals use 13 spectral channels in the 1500–4630 cm⁻¹ and the N₂O retrievals use 46 spectral channels in the 1183–4725 cm⁻¹ region. The Smithsonian Astrophysical Observatory (SAO) [Johnson *et al.*, 1995] far-infrared spectrometer (FIRS)-2 is an FTIR spectrometer which measures the limb emission at mid- and far-infrared wavelengths between 6 and 120 μm with a 0.004 cm⁻¹ resolution. The H₂O retrievals use 26 rotational transitions in both the far and mid infrared channels between 80 and 480 cm⁻¹. The transitions at higher frequency tend to add most of the weight to the retrievals in the upper troposphere and lower stratosphere, while the lower frequency transitions give more weight in the middle and upper stratosphere. The N₂O retrievals use 33 micro-windows in the ν_2 ro-vibrational band between 549 and 590 cm⁻¹. The vertical range is 8–40 km with a vertical resolution of 2–3 km. The JPL Submillimeterwave Limb Sounder-2 (SLS-2), an updated version of the instrument described by Stachnik *et al.* [1999], is a cryogenic heterodyne spectro-radiometer which measures the limb emission near 640 GHz with high resolution (2 MHz minimum channel width) for a number of species including N₂O. The vertical range is 15–45 km with a vertical resolution of 2–3 km below the balloon float altitude and 5–6 km above.

3.3.3. Ft. Sumner Comparisons The closest matching MLS profiles satisfy the coincidence criteria of $\pm 1^\circ$ in latitude, $\pm 12^\circ$ in longitude, and ± 12 hours with respect to the balloon measurement locations.

September 17, 2004 Figure 24 shows the N₂O comparison for the September 17, 2004 OMS flight (LACE). The MLS N₂O data show good agreement with respect to the 1- σ uncertainties and, except for the 46–32 hPa pressure levels, which are biased slightly low, the overall shape of the LACE measurements is well represented.

September 23–24, 2004 Figure 25 shows the H₂O and N₂O comparisons for the September 23–24, 2004 BOS flight (JPL MkIV and FIRS-2). The MLS H₂O data show good agreement with both MkIV and FIRS-2 within the 1- σ uncertainties for pressures ≤ 46 hPa. At 68–56 hPa MLS is biased low by ~ 0.3 ppmv and at 32–26 hPa an oscillation is apparent. The MLS N₂O data show good agreement with the MkIV data within the 1- σ uncertainties and capture the overall shape of the MkIV measurements. There is generally good agreement with the slope of the FIRS-2 data, but

FIRS-2 does not show the rise in N₂O at 32–10 hPa that is clearly seen by both MLS and MkIV. The N₂O feature is consistent with a dip in H₂O at the same levels as seen by all three instruments.

September 29, 2004 Figure 26 shows the N₂O comparison for the September 29, 2004 OMS flight (CWAS). The MLS N₂O data show reasonable agreement with the CWAS measurements although this particular comparison is 890 km distant.

September 20–21, 2005 Figure 27 shows the H₂O and N₂O comparisons for the September 20–21, 2005 BOS flight (JPL MkIV, FIRS-2, SLS-2). The MLS H₂O data show good agreement with the MkIV measurements with an overall slight low bias of ~ 0.3 ppmv for pressures ≤ 68 hPa and there is a reasonable comparison with the shape of the FIRS-2 data which shows a slight high bias ~ 0.3 ppmv relative to MkIV. At 32–26 hPa an oscillation is apparent in the MLS data. The MLS N₂O data show good agreement with the MkIV data within the $1\text{-}\sigma$ uncertainties throughout the pressure range. There is also good agreement with FIRS-2 for pressures < 68 hPa and these three instruments clearly show the rise in N₂O at 32–10 hPa. There is generally good overall agreement with the slope of the SLS-2 data, but SLS-2 does not show the N₂O feature seen by the other instruments. The N₂O feature is consistent with a dip in H₂O at the same levels as seen by MLS and MkIV.

4. Summary and Conclusions

The quality and reliability of the Aura MLS H₂O and N₂O measurements have been presented for the version 2.2 (v2.2) dataset which is expected to form the “definitive” version of the MLS data for the next several years. Version 2.2 is the second public release of MLS data and has been used to process the incoming data stream since March 2007. Reprocessing of the data collected since MLS became operational in August 2004 is also in progress using the v2.2 algorithms. These processing streams have the specific version name v2.21 and include a minor software patch applied to an earlier version v2.20 that corrects the handling of MLS Level 1 radiances flagged as bad data. We refer to both these versions collectively as version 2.2. For this validation effort, 93 days of v2.20 data covering late 2004 to early 2007 were processed with an emphasis on special months or days of interest for validation (including campaigns). The impacts of the various sources of systematic error have been estimated by a comprehensive set of retrieval simulations. Comparisons with correlative datasets from ground-based, balloon and satellite platforms operating in the uv/visible, infrared and microwave regions of the spectrum have been performed.

H₂O The stratospheric and mesospheric v2.2 H₂O data have been improved over v1.5 by providing higher vertical resolution in the lower stratosphere and better precision above the stratopause. However, a fine-scale oscillation in the v2.2 H₂O retrievals, possibly arising from the gain compression effect described in Section 2.6, causes the 31.6 hPa (26.1 hPa) level to be persistently low (high) by ~ 0.4 ppmv (8%). Table 2 summarizes the main characteristics of the MLS v2.2 H₂O product. The single-profile precision is $\sim 0.2\text{--}0.3$ ppmv (4–9%) and the vertical resolution is $\sim 3\text{--}4$ km in the stratosphere. The precision and vertical resolution become worse with increasing height above the stratopause. Over the pressure range 0.1–0.01 hPa the precision degrades from 0.4–1.1 ppmv (6–34%) and the vertical resolution degrades to $\sim 12\text{--}16$ km. The accuracy estimated from the systematic uncertainty analysis in Section 2.6 is 0.2–0.5 ppmv (4–11%) in the pressure range 68–0.01 hPa. The scientifically useful range of the H₂O data is from 316–0.002 hPa. The results of statistical comparisons with correlative data sources show good agreement (apart from the 31.6–26.1 hPa levels which show an additional $\pm 8\%$ bias) : ACE-FTS $\pm 5\%$ for pressures 68–0.004 hPa; HALOE +2% to +10% for pressures 68–1.5 hPa; SAGE II +5% to +10% for pressures 68–4.6 hPa; POAM II -3% to -17% for pressures 68–1 hPa; MIPAS -10% to 0% for pressures 22–0.68 hPa; WVMS $\pm 5\%$ for pressures 3.2–0.15 hPa. The above values are consistent with the corresponding published biases for HALOE, SAGE II, POAM and WVMS. Individual collocated profile comparisons with the JPL MkIV and FIRS-2 balloon measurements show generally good agreement.

N₂O Substantial improvement has been achieved in the v2.2 N₂O data over v1.5 by reducing the significant low bias in the stratosphere that was reported in *Froidevaux et al.* [2006] and eliminating unrealistically high biased mixing ratios in the polar regions. Table 3 summarizes the main characteristics of the MLS v2.2 N₂O product. The single-profile precision is $\sim 13\text{--}16$ ppbv (7–38%) and the vertical resolution is $\sim 4\text{--}5$ km for the pressure range 46–4.6 hPa. The accuracy estimated from the systematic uncertainty analysis in Section 2.6 is 3–32 ppbv (9–14%). The precision, resolution and accuracy become worse at higher pressures and for the 100–68 hPa levels the precision is $\sim 20\text{--}25$ ppbv (8–9%), the vertical resolution is $\sim 5\text{--}6$ km, and the estimated accuracy is 32–70 ppbv (13–25%). The scientifically useful range of the N₂O data is from 100–1 hPa. The results of statistical comparisons with correlative data sources show good agreement : ACE-FTS $\pm 5\%$ for pressures 100–1 hPa; MIPAS $\pm 5\%$ for pressures 32–1 hPa; Odin/SMR 0% to -5% for pressures 68–4.6 hPa and -10% at 100 hPa. Individual collocated profile comparisons with the LACE, CWAS, JPL

MkIV, JPL SLS-2 and FIRS-2 balloon measurements show generally good agreement.

We have provided several quality control metrics in the MLS Level 2 files as discussed in Section 2.2. To select data for scientific studies from the MLS v2.2 H₂O and N₂O products one should ensure that :

1. the precision value for a data point is positive,
2. the ‘Status’ field for the profile is even,
3. the ‘Quality’ field for the profile is >0.9 for H₂O or >0.5 for N₂O,
4. the ‘Convergence’ field for the profile is <1.55 for N₂O. This test is not required for H₂O.

Validation of the Aura MLS measurements is an ongoing process that will continue as more v2.2 data become available and enable opportunities for cross-comparisons with the recent January/February 2007 balloon flights from Kiruna, Sweden, active satellite missions and new deployments of instruments throughout the International Polar Year. Version 3 algorithms will address the problem of the oscillation in the H₂O retrievals at 32–26 hPa and the retrieval of N₂O may be extended to 147 hPa through the use of the 190-GHz measurements.

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Table 1. Meaning of bits in the ‘Status’ field.

Bit	Value ^a	Meaning
0	1	Flag: Do not use this profile (see bits 8–9 for details)
1	2	Flag: This profile is ‘suspect’ (see bits 4–6 for details)
2	4	Unused
3	8	Unused
4	16	Information: This profile may have been affected by high altitude clouds
5	32	Information: This profile may have been affected by low altitude clouds
6	64	Information: This profile did not use GEOS-5 temperature a priori data
7	128	Unused
8	256	Information: Retrieval diverged or too few radiances available for retrieval
9	512	Information: The task retrieving data for this profile crashed (typically a computer failure)

^a‘Status’ field in L2GP file is total of appropriate entries in this column.

Table 2. Summary of the MLS v2.2 H₂O product

Pressure hPa	Resolution		Precision ^b		Accuracy ^c		Comments
	Vert. km	× Horiz. ^a km	ppmv	%	ppmv	%	
0.001	—	—	—	—	—	—	Not recommended for scientific use
0.002	13 ×	320	1.9	180	0.3	34	
0.004	13 ×	360	1.5	82	0.3	16	
0.010	12 ×	390	1.1	34	0.4	11	
0.022	12 ×	420	0.8	18	0.4	9	
0.046	16 ×	430	0.6	10	0.5	8	
0.10	14 ×	440	0.4	6	0.5	8	
0.22	6.7 ×	420	0.3	5	0.4	7	
0.46	5.5 ×	410	0.3	4	0.5	6	
1.00	4.6 ×	410	0.3	4	0.3	4	
2.15	4.0 ×	380	0.2	4	0.3	5	
4.64	3.6 ×	320	0.2	4	0.4	7	
10.0	3.3 ×	280	0.2	4	0.5	9	
21.5	3.2 ×	290	0.2	4	0.4	7	
46.4	3.1 ×	240	0.3	6	0.2	4	
68.1	3.2 ×	220	0.3	8	0.2	6	
≥82.3	—	—	—	—	—	—	

^aHorizontal resolution in the along-track direction; across-track resolution is ~ 7 km and the separation between adjacent retrieved profiles along the measurement track is 1.5° great circle angle (~ 165 km).

^bPrecision on individual profiles; $1\text{-}\sigma$ estimate from the Level-2 algorithms.

^cSystematic uncertainty; $2\text{-}\sigma$ estimate of the probable magnitude.

Table 3. Summary of the MLS v2.2 N₂O product

Pressure hPa	Resolution Vert. × Horiz. ^a km	Precision ^b		Accuracy ^c		Comments
		ppbv	%	ppbv	%	
≤0.68	—	—	—	—	—	Not recommended for scientific use
1.00	6.5 × 300	14	250	0.6	12	
2.15	4.9 × 340	15	110	1.2	9	
4.64	4.1 × 370	14	38	3	9	
10.0	3.8 × 430	13	16	7	9	
21.5	4.1 × 490	13	9	19	13	
46.4	4.3 × 540	16	7	32	14	
68.1	5.6 × 590	20	8	32	13	
100	5.2 × 620	25	9	70	25	
147	—	—	—	—	—	Not recommended for scientific use
≥215	—	—	—	—	—	Not retrieved

^aHorizontal resolution in the along-track direction; across-track resolution is ~3 km and the separation between adjacent retrieved profiles along the measurement track is 1.5° great circle angle (~165 km).

^bPrecision on individual profiles; 1- σ estimate from the Level-2 algorithms.

^cSystematic uncertainty; 2- σ estimate of the probable magnitude.

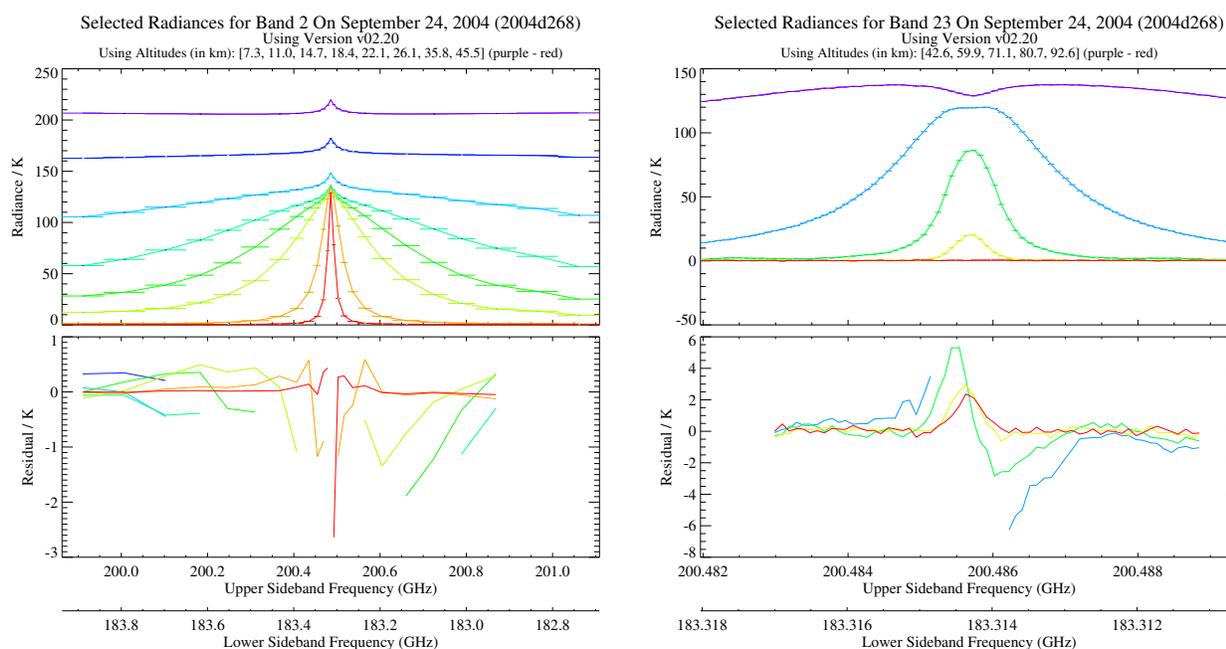


Figure 1. Sample radiance spectrum and residuals from the Aura MLS 190-GHz radiometer for band 2 (Left) and the DACS for band 23 (Right). Band 23 occupies a narrow spectral region at the center of band 2. (Top panels) Global average radiances for a representative day (24 September 2004) for selected tangent point altitudes (purple–red). The widths of the spectral channels are denoted by horizontal bars. (Bottom panels) Global average radiance residuals for the fit achieved by the Level 2 retrieval algorithm. Gaps along the frequency axis of the residual plots indicate channels that are not used in the retrieval. The radiance noise averaged down by the number of samples is insignificant compared to the residual spectrum.

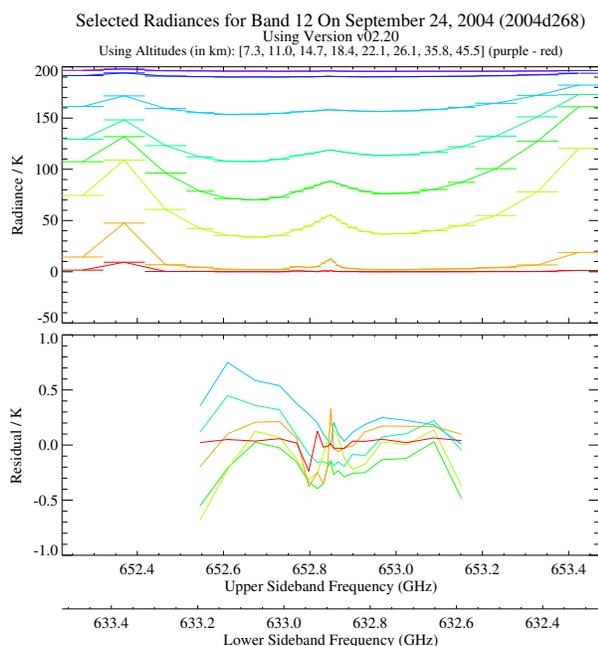


Figure 2. Sample radiance spectrum and residuals from the Aura MLS 640-GHz radiometer for band 12. Description of panels as in Figure 1.

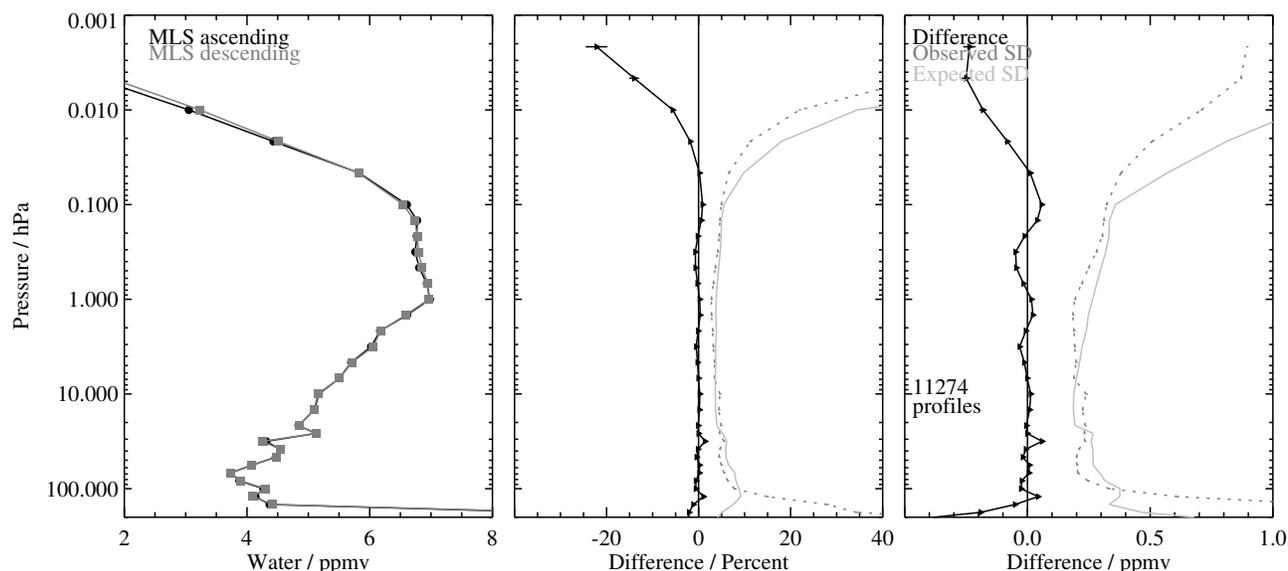


Figure 3. Comparison of MLS v2.2 H₂O ascending and descending orbit matching profile pairs in the latitude range 50° S–50° N averaged over 92 days. (Left) Ensemble mean profiles for ascending (black circles) and descending (dark gray squares) orbit matches. (Center) Mean percentage difference profiles (black triangles) between the ascending and descending orbits; the percentage standard deviation about the mean difference (Observed SD; dark gray dashed line) and the percentage root sum square of the theoretical precisions (Expected SD; light gray solid line) calculated by the retrieval algorithms for the two datasets. (Right) As the center panel except plotted in mixing ratio units. In this figure the SD values have been scaled by $1/\sqrt{2}$ and hence the observed SD represents the statistical repeatability of the measurements and the expected SD represents the theoretical 1- σ precision for a single profile.

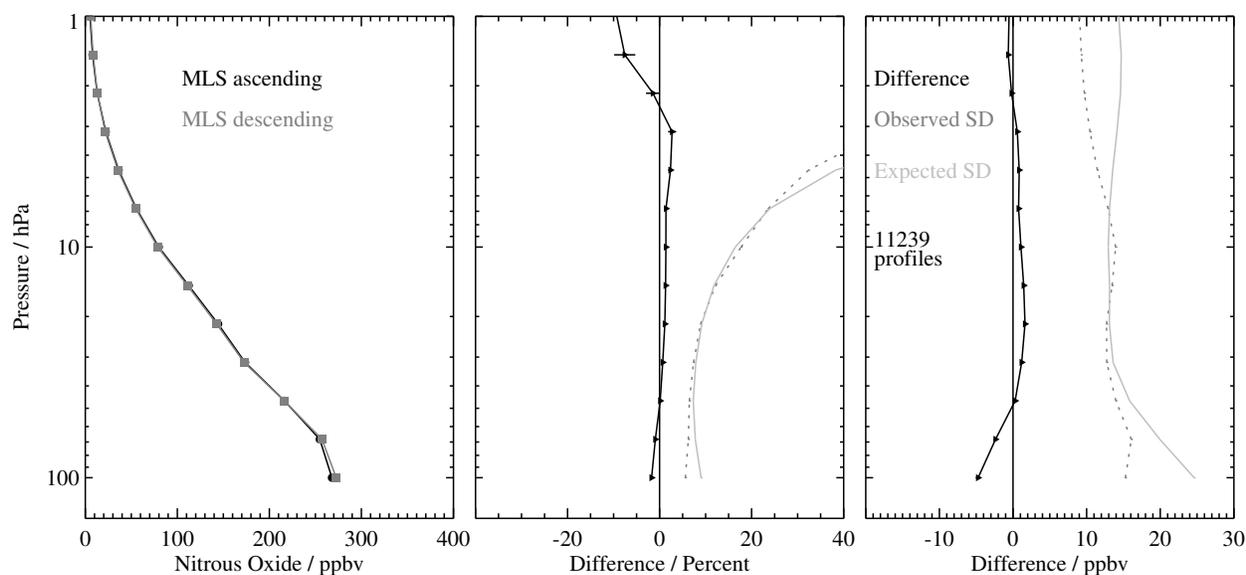


Figure 4. As Figure 3 except for N₂O.

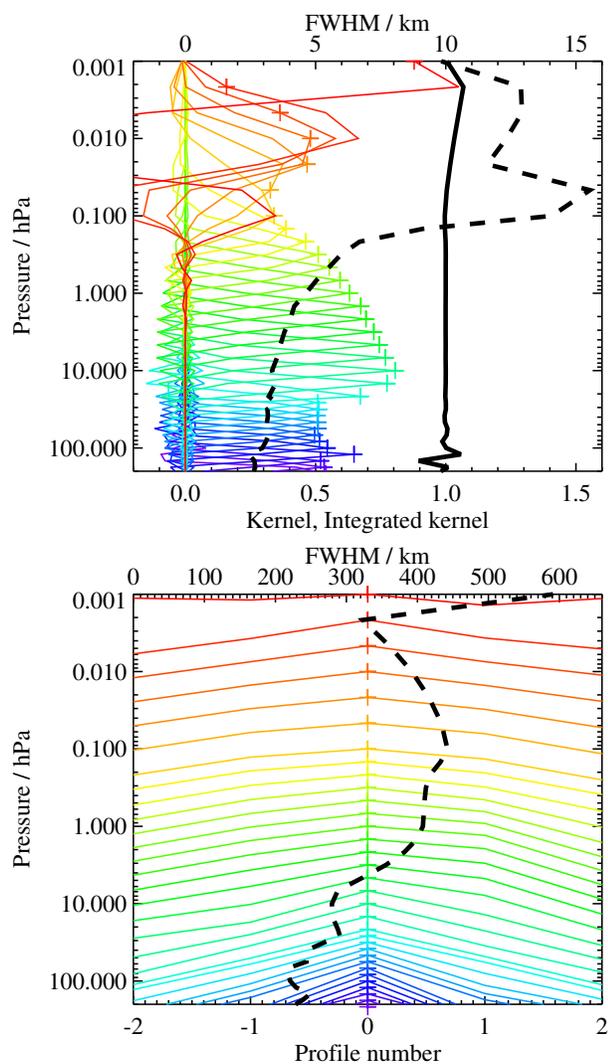


Figure 5. Typical representations of the two-dimensional (vertical and horizontal along-track) averaging kernels for the MLS H_2O retrieval at 35°N . The colored lines show the kernels as a function of the retrieval level. These kernels indicate the region of the atmosphere which contributes to the retrieval level denoted by the plus symbols. The solid black line shows the integrated area under each of the colored curves; values near unity indicate that almost all the information at that level was contributed by the measurement system, whereas lower values indicate increasing contributions from the a priori information. The dashed black line indicates the vertical (or horizontal) resolution as determined from the full width at half-maximum (FWHM) of the averaging kernel approximately scaled into kilometers (top axis). (Top) Vertical averaging kernels (integrated in the horizontal dimension for 5 along-track profiles) and resolution. (Bottom) Horizontal averaging kernels (integrated in the vertical dimension) and resolution. The averaging kernels are scaled such that a unit change is equivalent to one decade in pressure. Profiles are spaced at 1.5° great circle angle corresponding to 165 km along the orbit track.

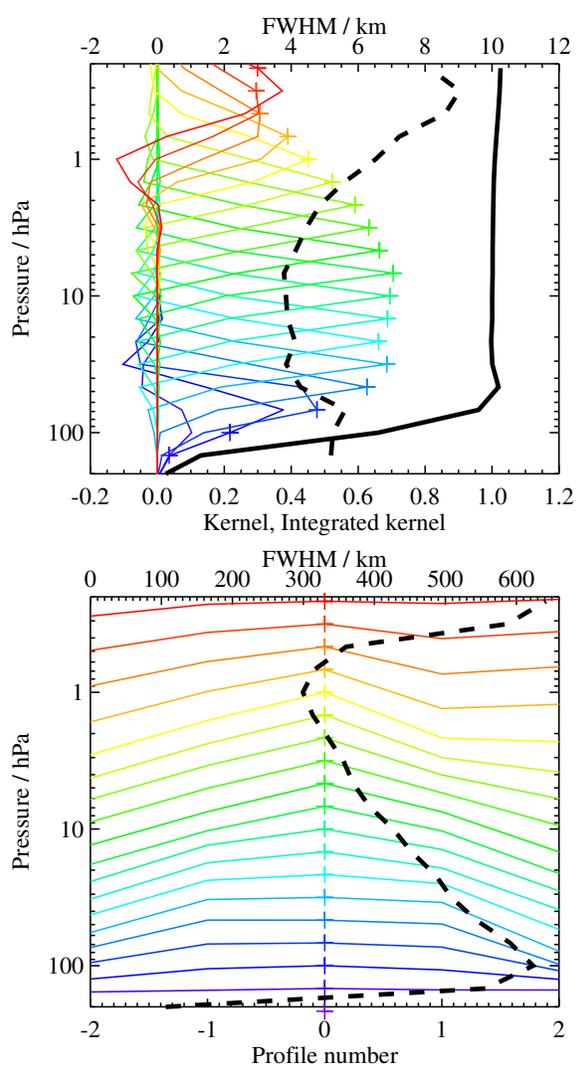


Figure 6. As for Figure 5 but showing the MLS N_2O retrieval averaging kernels.

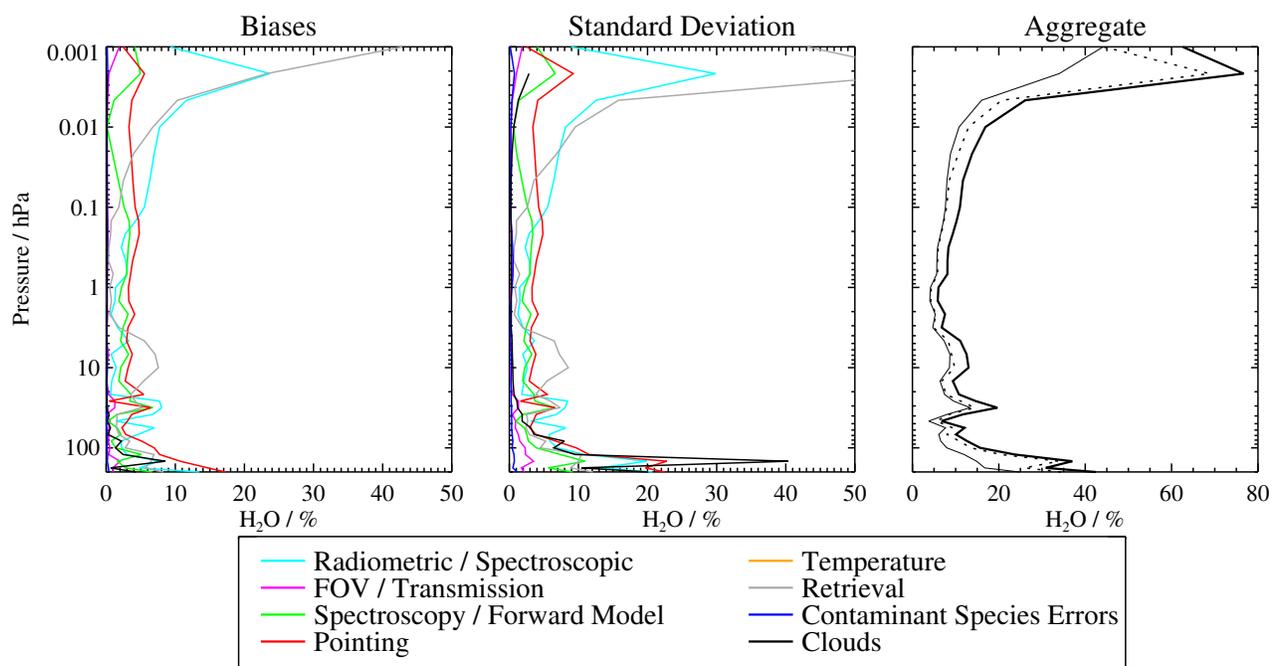


Figure 7. The estimated impact ($2\text{-}\sigma$) of various families of systematic uncertainty on the MLS H_2O observations with each family denoted by a different colored line. Cyan lines denote uncertainties in MLS radiometric and spectral calibration. Magenta lines show uncertainties associated with the MLS field of view and antenna transmission efficiency. Red lines depict errors associated with MLS pointing uncertainty. The impacts of uncertainties in spectroscopic databases and forward model approximations are denoted by the green line, while those associated with retrieval formulation are shown in gray. The gold lines indicate uncertainty resulting from errors in the MLS temperature product, while the blue lines show the impact of similar ‘knock on’ errors in other species. Cloud impacts are shown as the thin black line. (First panel) Estimated bias. (Center panel) Standard deviation about the bias. (Right panel) Root sum square of all the possible biases (thin solid line), all the additional scatter (thin dotted line), and the RSS sum of the two (thick solid line)

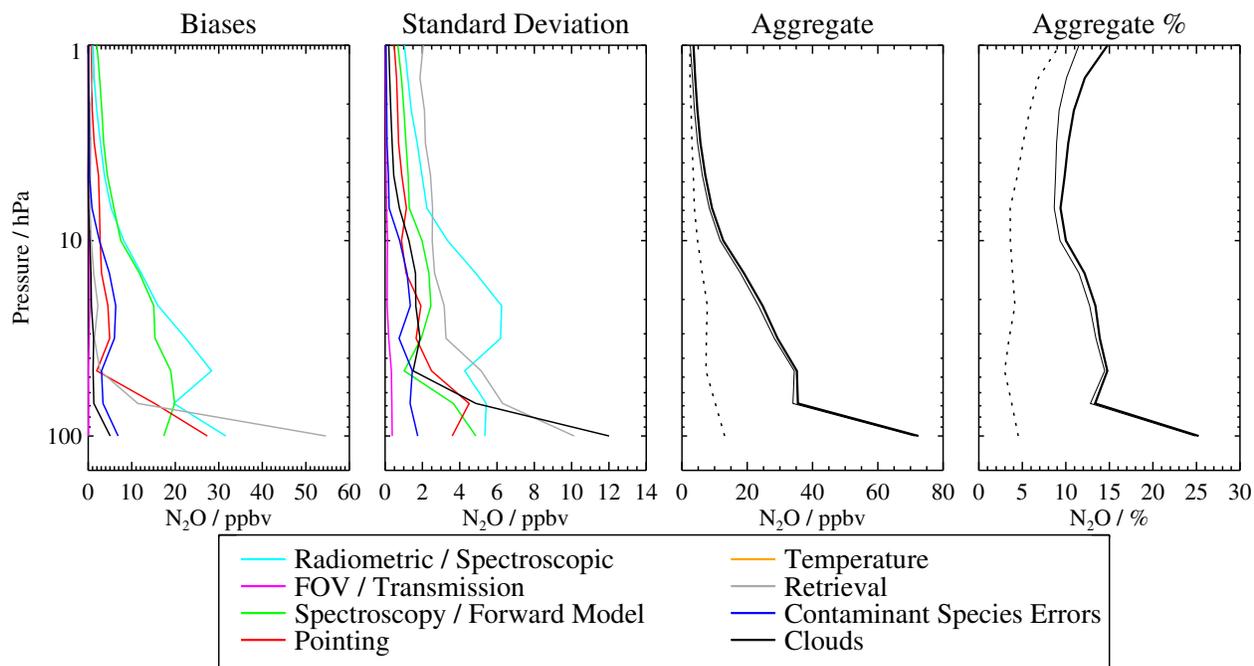


Figure 8. As for Figure 8 but showing the MLS N_2O error sources

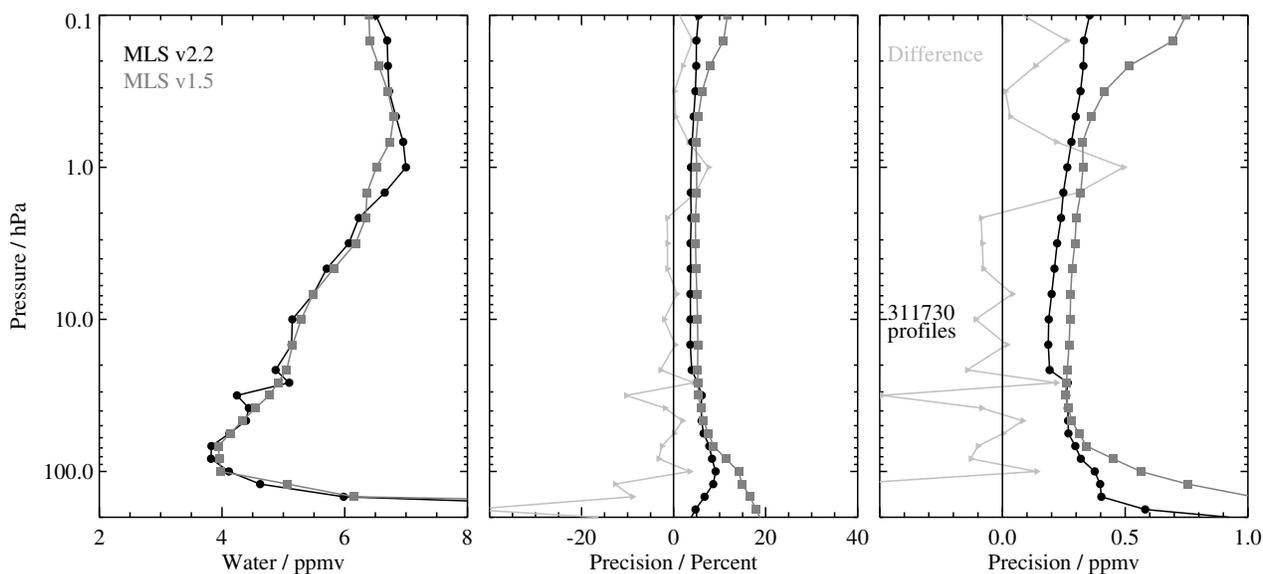


Figure 9. Comparison of MLS v2.2 H_2O with v1.5 averaged over 92 days. (Left) Ensemble global mean profiles for v2.2 (black circles) and v1.5 (dark gray squares). (Center) Mean percentage difference profiles between v2.2 and v1.5 ($v2.2 - v1.5$; light gray triangles) and the percentage theoretical precision for v2.2 (black circles) and v1.5 (dark gray squares). (Right) As the center panel except plotted in mixing ratio units.

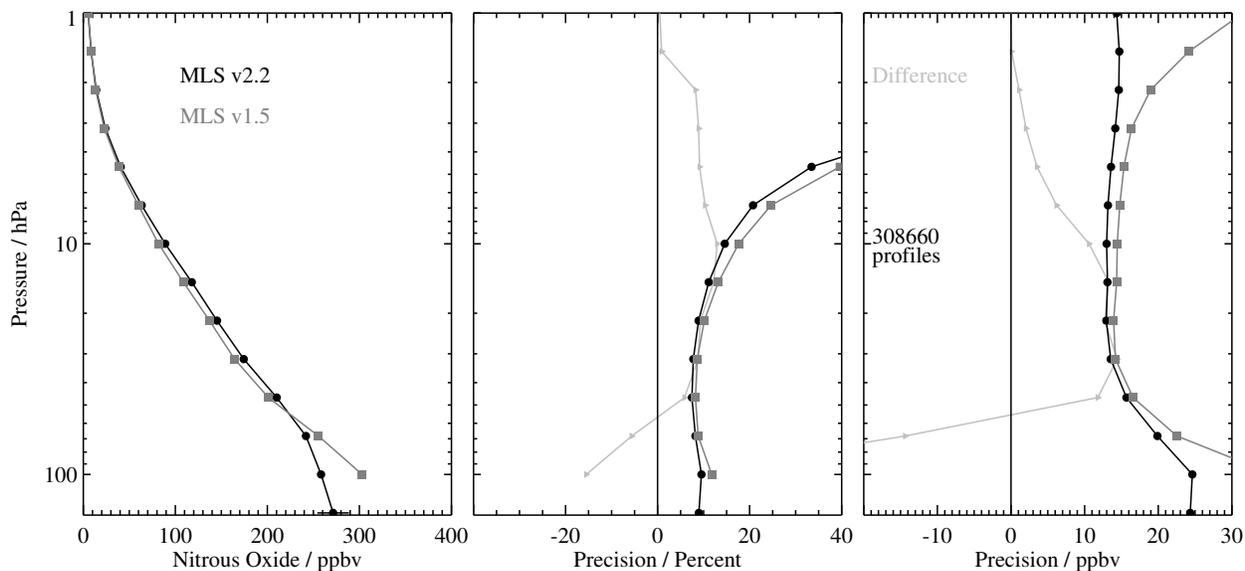


Figure 10. As Figure 9 except for N_2O .

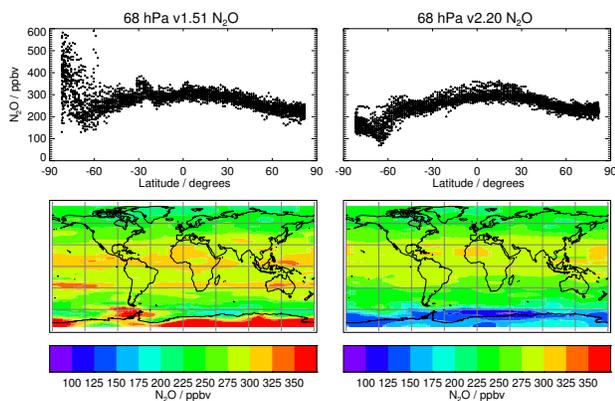


Figure 11. Comparison of MLS v2.2 N_2O (Right panels) to MLS v1.5 (Left panels) on September 17, 2005 for the 68 hPa pressure surface. (Top panels) Scatter plots of the N_2O mixing ratio as a function of latitude. (Bottom panels) Gridded maps of the distribution of the N_2O mixing ratio. Anomalously high values of N_2O in the Southern Hemisphere polar vortex retrieved in the v1.5 processing have been eliminated in v2.2

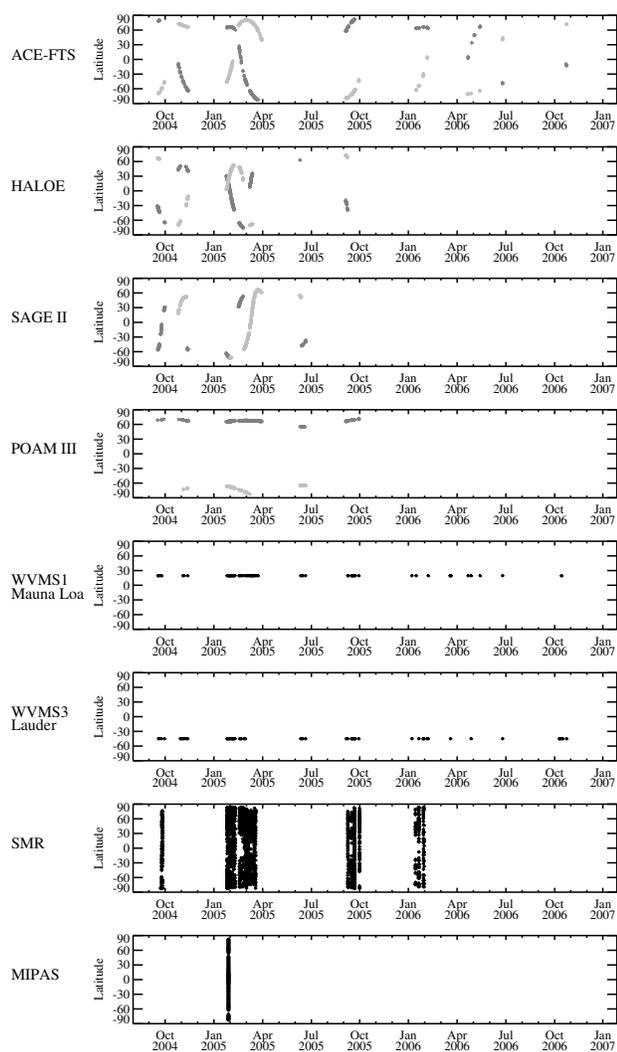


Figure 12. Sampling distributions in latitude and time of the collocated coincident matches of the v2.2 MLS data with the spaceborne and ground-based correlative instruments. For the solar occultation instruments the sunrise and sunset events are denoted by the dark-gray and light-gray symbols, respectively.

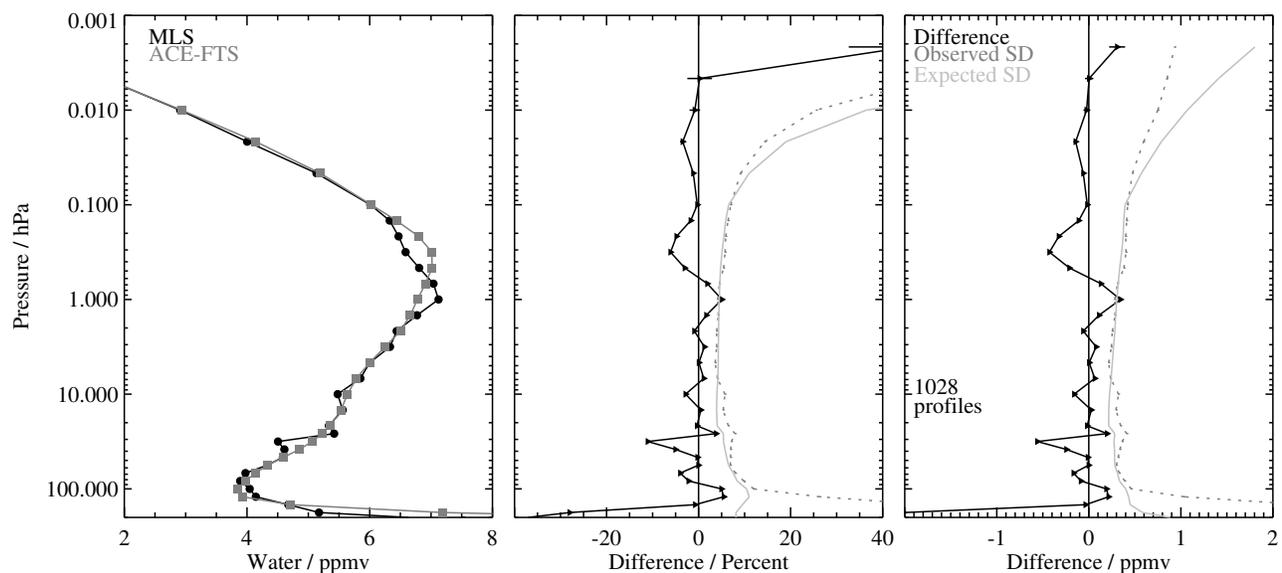


Figure 13. MLS H_2O compared to ACE-FTS averaged over 121 days of collocated data. (Left) Global ensemble mean profiles of the collocated matches for both instruments (MLS black circles; ACE-FTS dark gray squares). (Center) Mean percentage difference profiles between the two measurements (MLS–ACE-FTS) (black triangles); standard deviation about the mean differences (Observed SD; dark gray dashed line) and the percentage root sum square of the precisions on both instrument measurements (Expected SD; light gray solid line). (Right) As the center panel except plotted in mixing ratio units.

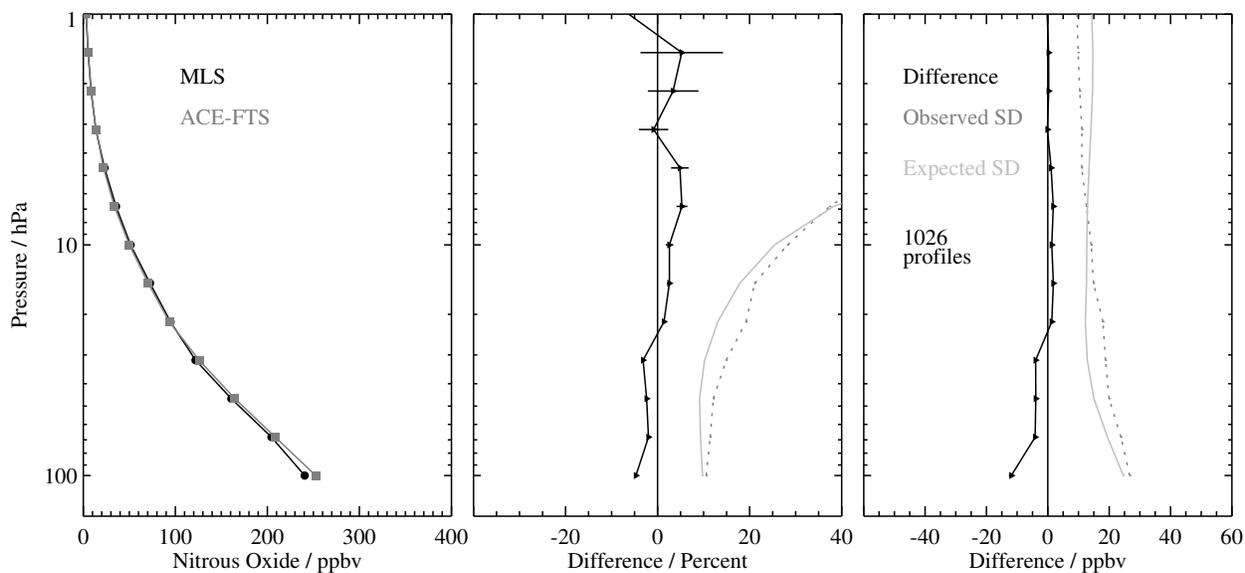


Figure 14. As Figure 13 except for ACE-FTS N_2O

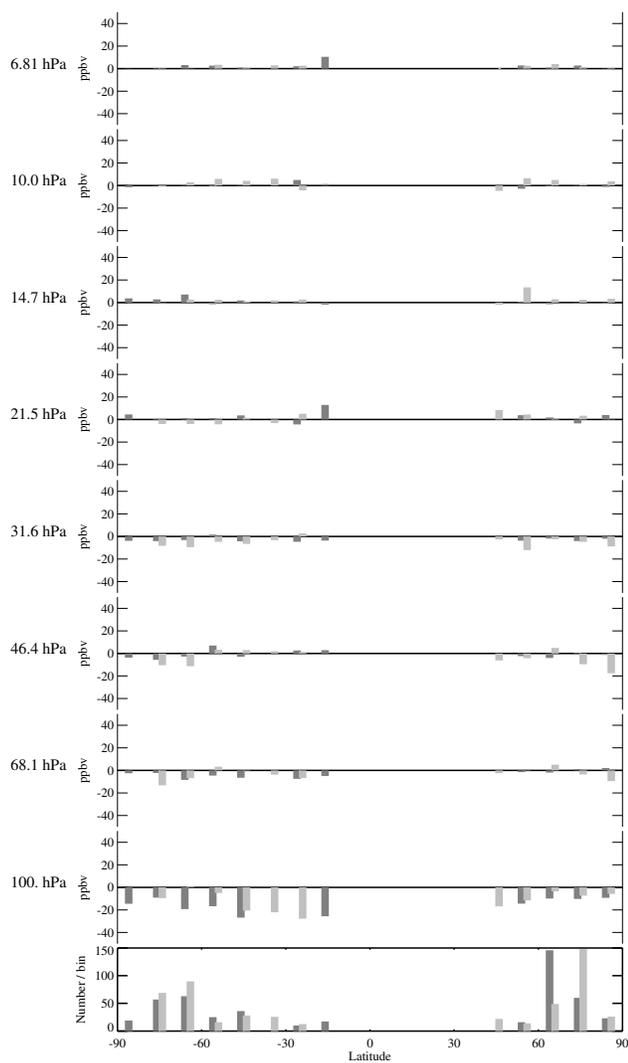


Figure 15. MLS N_2O compared to ACE-FTS for 121 days of collocated data. Distributions of the mean (MLS–ACE-FTS) N_2O mixing ratio differences in 10° latitude bins for sunrise (dark gray) and sunset (light gray) collocated profiles. Only latitude bins containing at least 10 collocated profiles are plotted. The bottom panel shows the number of sunrise/sunset occultations in each latitude bin.

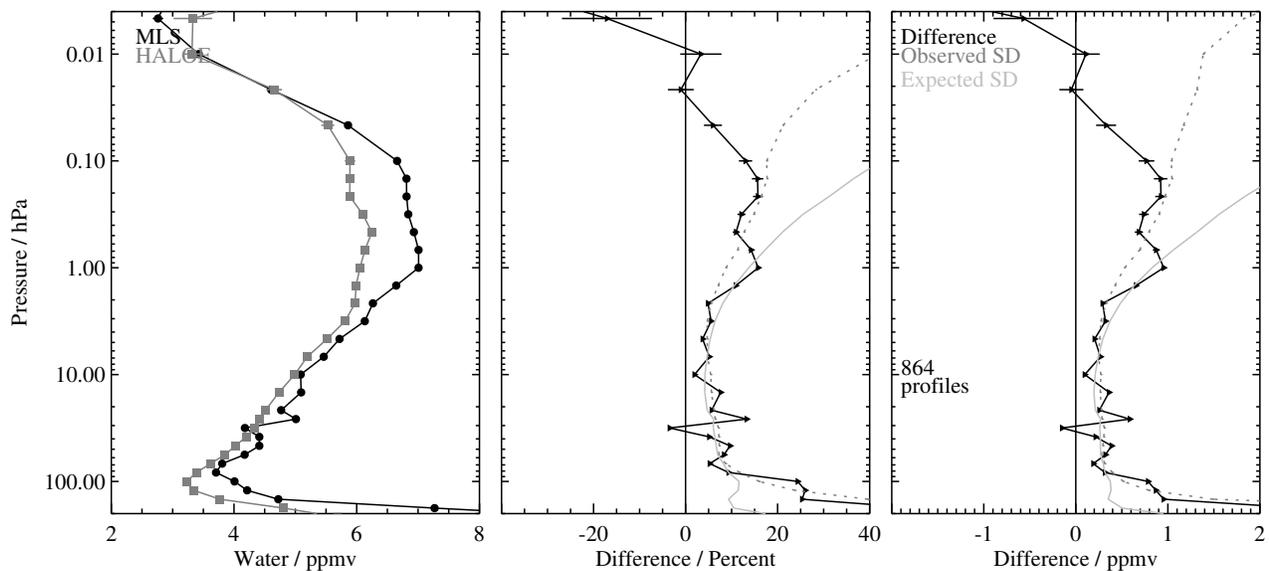


Figure 16. As Figure 13 except for HALOE H₂O averaged over 53 days of collocated data.

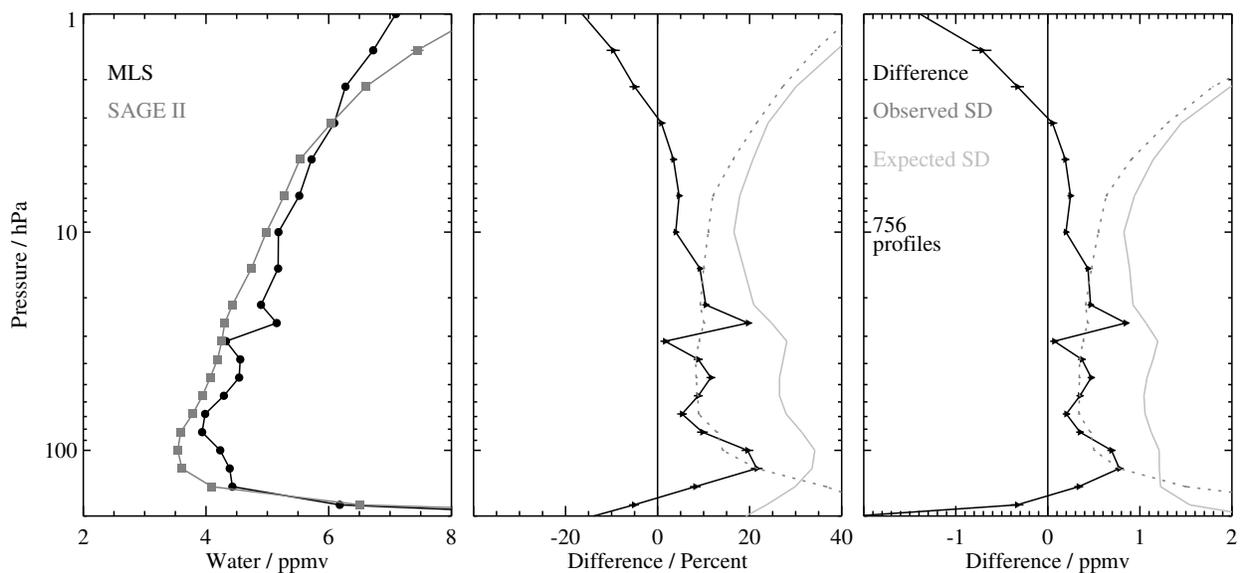


Figure 17. As Figure 13 except for SAGE II H₂O averaged over 87 days of collocated data.

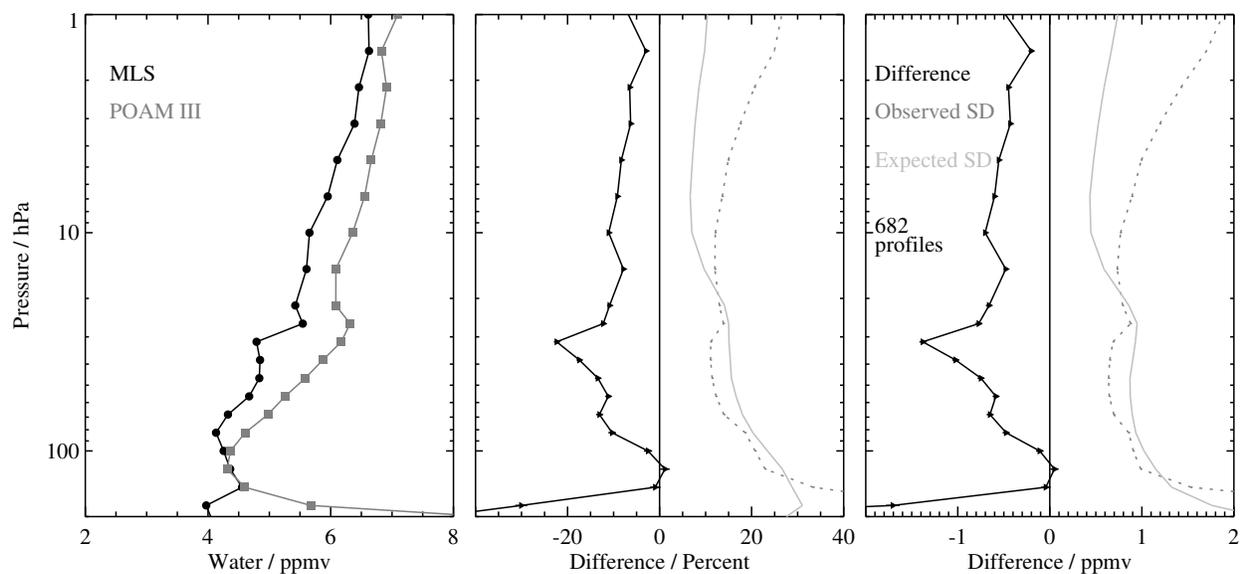


Figure 18. As Figure 13 except for POAM III H₂O averaged over 92 days of collocated data.

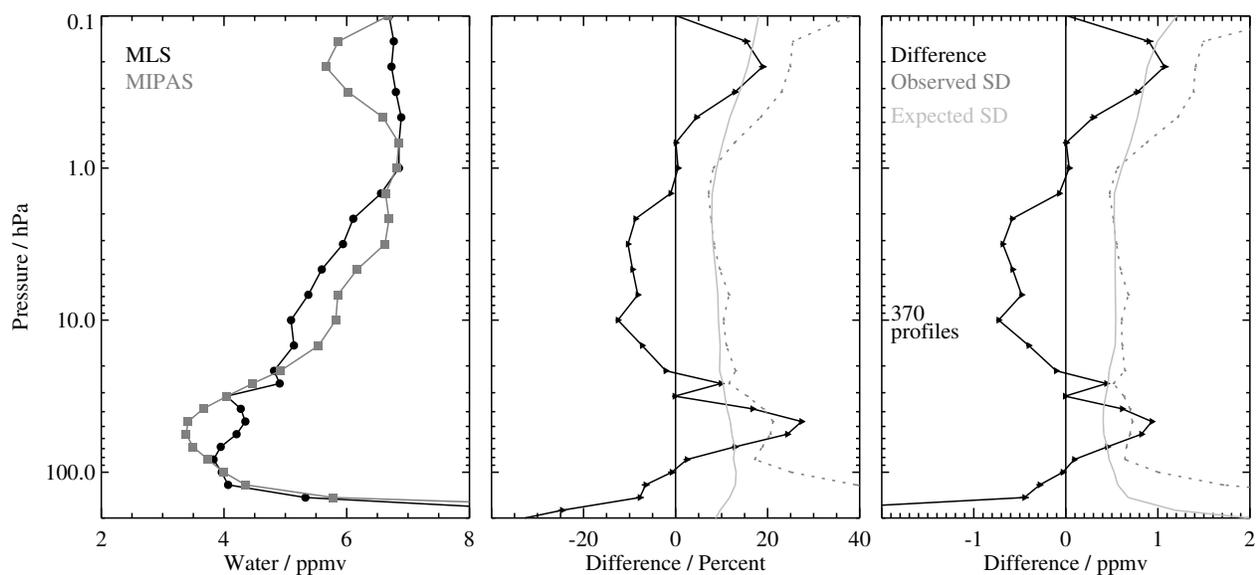


Figure 19. As Figure 13 except for MIPAS H₂O on January, 28 2005.

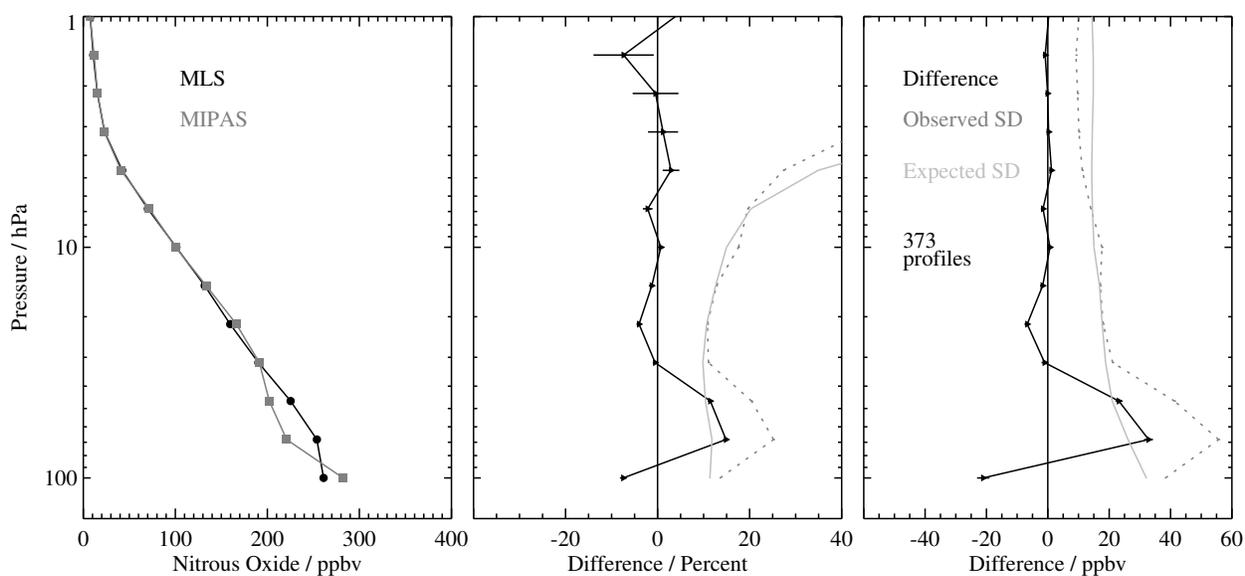


Figure 20. As Figure 13 except for MIPAS N₂O on January, 28 2005.

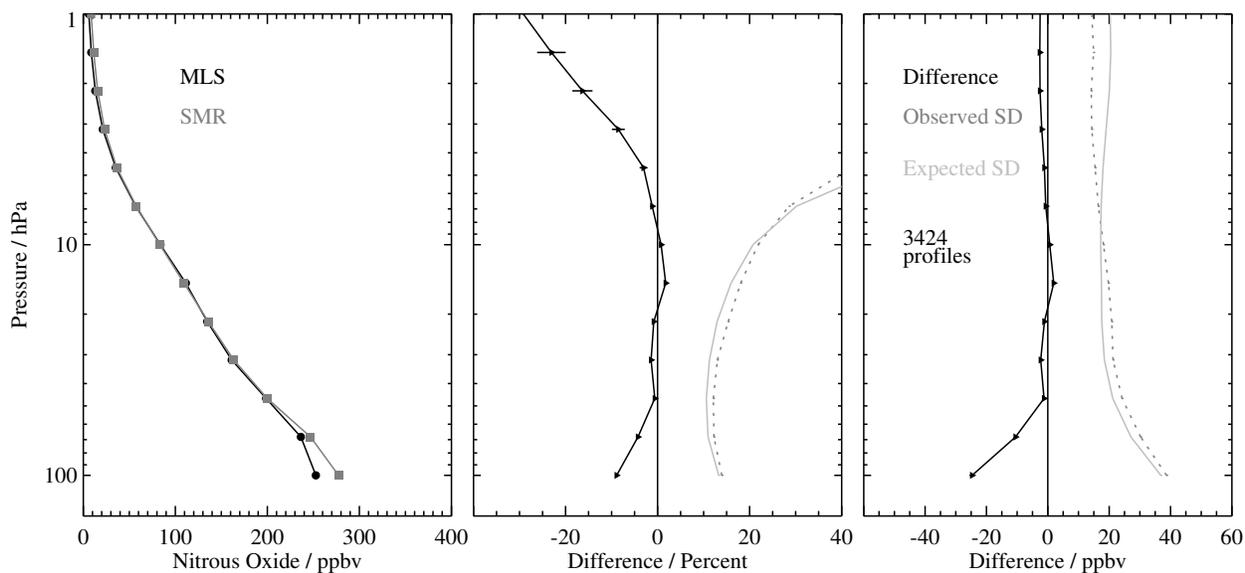


Figure 21. As Figure 13 except for SMR N₂O averaged over 49 days of collocated data.

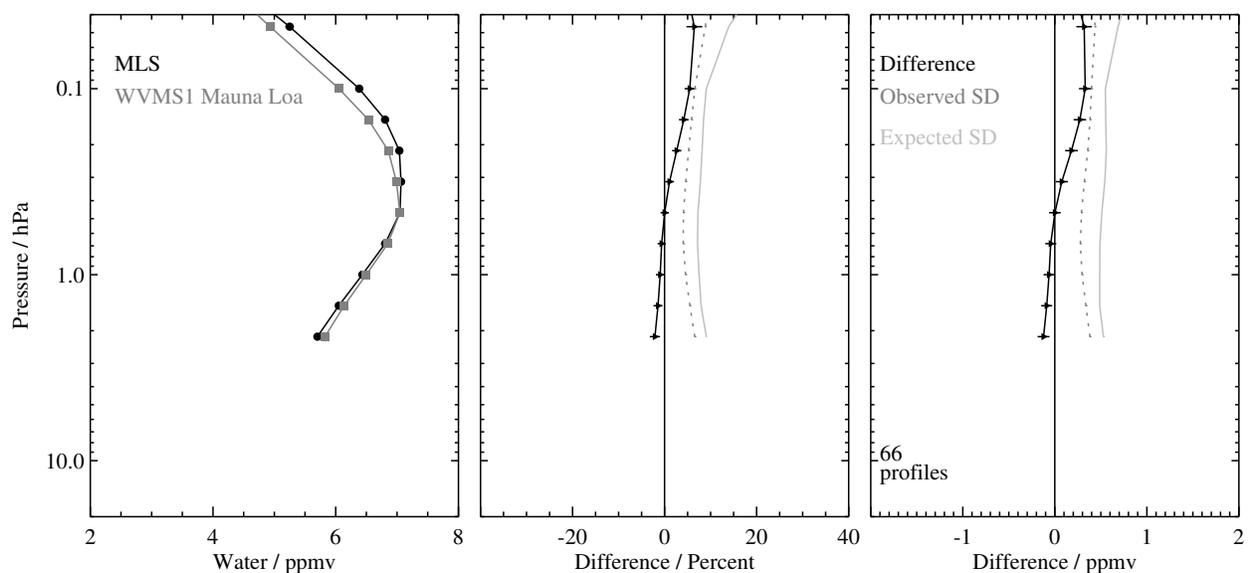


Figure 22. As Figure 13 except for WVMS Mauna Loa H₂O averaged over 66 days of collocated data. The MLS retrievals have been convolved with the WVMS Mauna Loa averaging kernels.

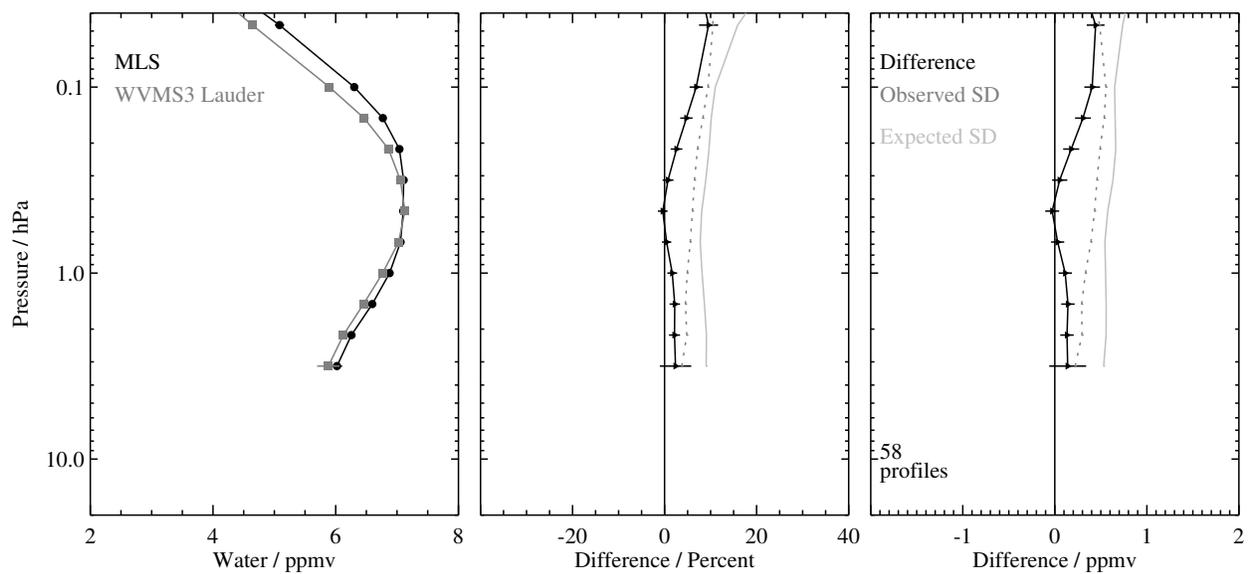


Figure 23. As Figure 13 except for WVMS Lauder H₂O averaged over 58 days of collocated data. The MLS retrievals have been convolved with the WVMS Lauder averaging kernels.

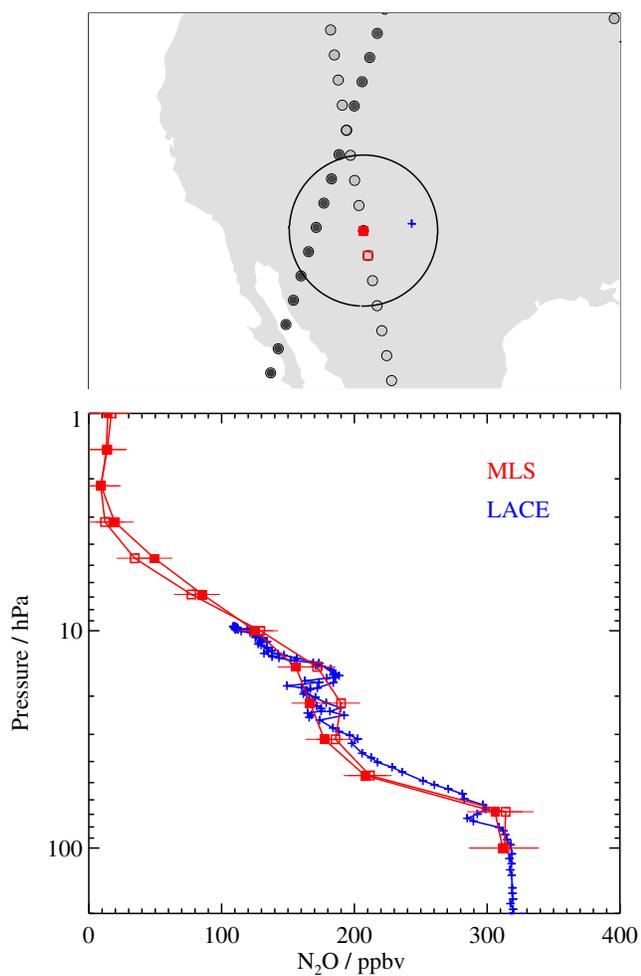


Figure 24. MLS N₂O ascending orbit overpass measurements (20:29 UT) compared to the LACE measurements (15:27–20:14 UT) from the OMS gondola flown from Ft. Sumner on September 17, 2004. The location map shows the MLS overpass ascending (light circles) and descending orbit (dark circles) tangent points. The two closest coincident MLS profiles (see text) are shown as filled (best match) and open red squares. The map scale is indicated by a 500 km radius locus centered on the best match. The correlative balloon instrument measurement locations are shown.

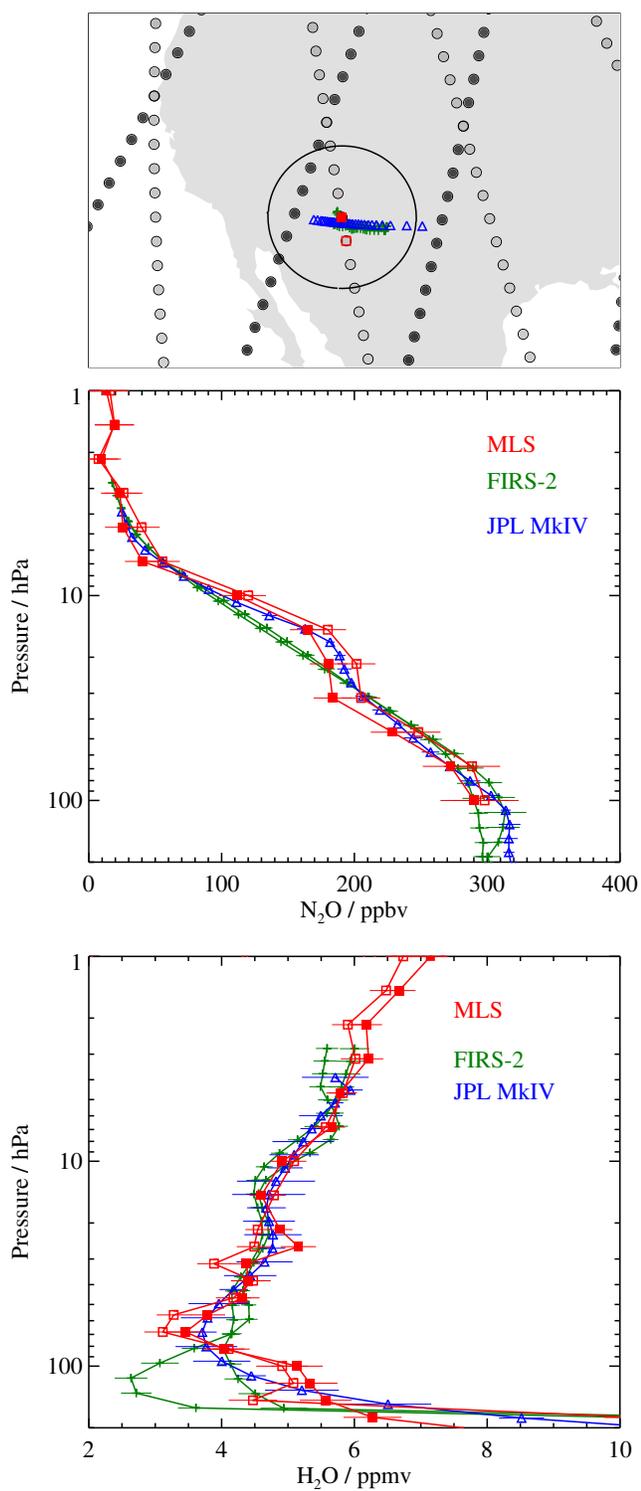


Figure 25. MLS N_2O and H_2O ascending orbit overpass measurements (September 23, 20:35 UT) compared to the FIRS-2 (September 24, 02:33, 04:54 UT) and JPL MkIV (September 24, 00:00–01:12 UT) measurements from the BOS gondola flown from Ft. Sumner on September 23–24, 2004. Location map details are as in Figure 24.

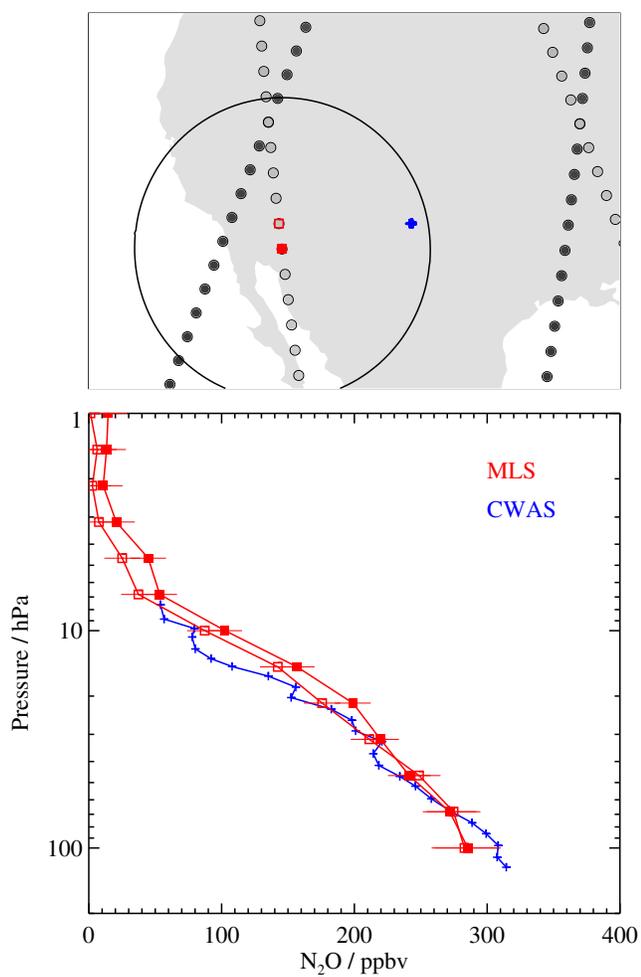


Figure 26. MLS N₂O ascending orbit overpass measurements (20:54 UT) compared to the CWAS measurements (16:37–20:09 UT) from the OMS gondola flown from Ft. Sumner on September 29, 2004. Location map details are as in Figure 24 except a 1000 km radius locus is centered on the closest matching MLS profile.

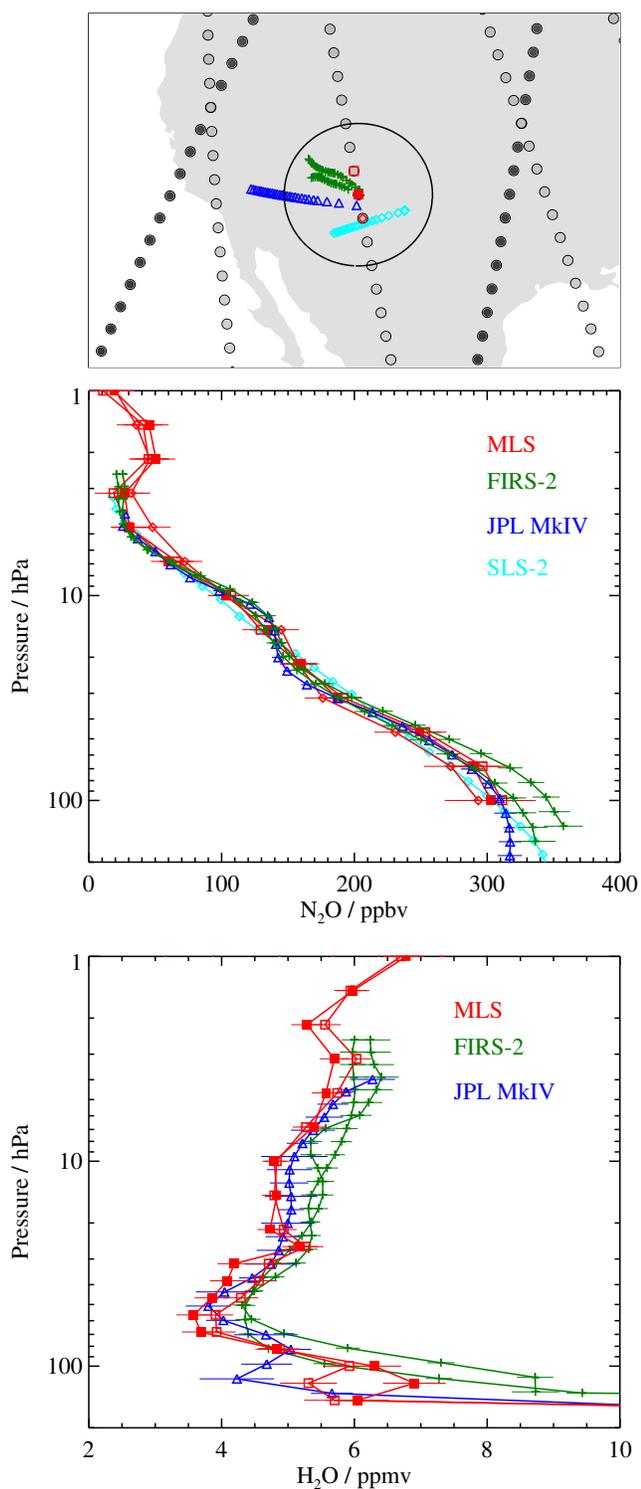


Figure 27. MLS N_2O and H_2O ascending orbit overpass measurements (September 20, 20:27 UT) compared to the FIRS-2 (September 20, 20:34, 21:44 UT), JPL MkIV (September 21, 00:43–01:47 UT) and SLS-2 (September 20, 17:50 UT) measurements from the BOS gondola flown from Ft. Sumner on September 20–21, 2005. Location map details are as in Figure 24 except an additional MLS profile match (red diamond symbol) for N_2O is shown which matches better the SLS-2 measurement locations.