JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 104, NO. D8, PAGES 9399–9412, APRIL 27, 1999

Validation of a new prototype water vapor retrieval for the UARS Microwave Limb Sounder

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Abstract. The UARS Microwave Limb Sounder (MLS) measured water vapor in the middle atmosphere between September 1991 and April 1993. The current version of the data, version 4, and its predecessor, version 3, have been used in many scientific studies. As part of the process of developing the next version of UARS MLS data, a new prototype retrieval for the stratosphere/mesosphere water vapor product was developed at the University of Edinburgh. The main improvements made were (1) corrections for systematic errors and (2) doubling of the vertical resolution of the retrieval grid. Initial results were sufficiently encouraging that the code was used to produce data for all UARS days on which the MLS 183 GHz radiometer was operational. This paper describes these data and examines their quality. Comparisons are made with the available correlative data and it emerges that the prototype agrees better with the correlative data than does version 4. Agreement with frost point hygrometers is excellent in the lower stratosphere and agreement with a ground-based microwave is satisfactory in the upper stratosphere and mesosphere. Agreement with two solar occultation instruments, Atmospheric Trace Molecular Spectroscopy Experiment (ATMOS) and Halogen Occultation Experiment (HALOE), is better than it was for earlier MLS versions but the prototype data are uniformly drier than both of these instruments. We compare the data with version 4, showing several features which are more clearly visible in the new prototype. These include seasonal cycles in the upper mesosphere and equatorial lower stratosphere.

1. Introduction

The Microwave Limb Sounder (MLS) is an instrument on the Upper Atmosphere Research Satellite (UARS). UARS was launched in September 1991 and is still operating at the time of writing, mid-1998, although stratosphere/mesosphere water vapor measurements ceased in April 1993. MLS is designed to measure temperature and the mixing ratios of several trace molecules in the stratosphere and mesosphere. It receives thermally emitted microwave radiation using a parabolic dish antenna whose field of view is scanned vertically across the Earth's limb. The incoming radiation is fed via a superheterodyne receiver into several filter banks or "bands" which are centered on the frequencies of rotational transitions of the target molecules. One filter bank (known as band 1) is targeted at two lines in the 60 GHz spin rotation band of the oxygen molecule. The mixing ratio of oxygen is known, so this bank is used to determine the temperature and the pressure of the point along the line of sight which is closest to the Earth. These pressures, known as tangent pressures, form the vertical grid for the radiance measurements. The other five banks are used to measure trace species mixing ratios. Further details are given by *Barath et al.*[1993].

This paper concentrates on the filter bank (band 5) which is centered on the 183.3 GHz transition of the water molecule. The data from these filters provide information on the water vapor content of the atmosphere between altitudes of 16 km and 90 km. The UARS project has already processed these data to give profiles of water vapor mixing ratio. Two versions of the MLS data, versions 3 and 4, have been released to the public and have been used in a number of scientific studies, summarized by *Waters et al.* [1998].

The version 3 water vapor product had a number of limitations and systematic errors which are described in detail by *Lahoz et al.* [1996]. One limitation was that the vertical resolution in the stratosphere was limited by the vertical grid onto which the mixing ratio was retrieved. The grid was chosen for computational speed and stability; the instrument is capable of better vertical resolution than the version 3 grid permits. Another limitation was that the retrieved product was controlled to a large extent by the a priori in the polar winter lower stratosphere. The second limitation was removed in version 4; the first was not. The lowest altitude at which water vapor was retrieved was 46 mbar in both versions.

Version 3 showed a slight positive bias of about 0.3 ppmv against most correlative measurements in the lower stratosphere. The magnitude of this bias became larger with altitude, culminating in an extremely large positive bias of 1.5–2.5 ppmv at 0.1 mbar. As a result, the MLS team recom-

Paper number 1998JD200113.
0148-0227/99/1998JD200113$09.00

mended that the data not be used at this altitude or above. In version 4 the bias in the lower stratosphere was somewhat reduced, to the point where MLS was 0.2 ppmv wetter than some instruments and less than 0.2 ppmv drier than others. The large biases in the lower mesosphere remained.

A problem with version 3 which Lahoz et al. did not discuss is that a strong systematic difference exists between the retrieved products on the ascending and descending legs of the UARS orbit. This problem occurs mainly at 0.1 mbar, above the highest level where use of the data was recommended. In version 4 this problem became worse, not better, although it was still largely confined to the mesosphere. Another artifact, noted by *Mote et al.* [1995], is that the retrieved water vapor values are affected by the UARS yaw cycle, particularly at 22 mbar.

The data described in this paper are a result of work done in order to find out what was necessary to produce a substantially improved water vapor product. There was a clear scientific requirement to improve the vertical resolution and to produce usable data at lower altitudes [*Mote et al.* 1995], so priority was given to these aims. The problem was known to be sufficiently nonlinear in the lower stratosphere that an iterative algorithm would be required. Furthermore, the version 3 and 4 retrievals suffered from poor closure, that is, radiances calculated from the retrieved products did not agree well with the radiances which were measured. In version 3 the difference between measured and calculated radiances was typically between 2 and 5 times larger than the measurement error [see *Lahoz et al.,* 1996, Figure 5]. This indicated that our modeling of the instrument and the radiative transfer in the atmosphere was not accurate enough.

Work began on a prototype retrieval program which addressed these problems, and results from a very early stage in this process were used in a study of the equatorial lower stratosphere [*Mote et al.,* 1996]. At that stage the program was too slow to process the whole data set, and the results had serious systematic biases, although the vertical resolution was improved and the seasonal cycles were realistic. Further work eliminated these biases and speeded up the code. The results at this point were sufficiently encouraging that the retrieval was run for one UARS yaw period and the results used in a study of the 4-day wave in the upper stratosphere [*Manney et al.,* 1998]. Following on from this, it was decided that the whole data set should be processed using this code so that more scientific studies could be pursued at the same time as further improvements were being made to the retrieval. The rest of this paper describes the resulting data and the method by which they were produced.

2. Description of Retrievals

The retrieval was done using optimal estimation (OE) [*Rodgers,* 1976]. This method is useful in any situation where we have a vector $\mathbf{x}$ that we wish to know but cannot measure and a vector $\mathbf{y}$ which we can measure and which is related to $\mathbf{x}$ by a known function F. It is usual to call $\mathbf{x}$ the state vector and $\mathbf{y}$ the measurement vector. An iterative version of OE, the inverse Hessian or Newtonian iteration method [*Rodgers,* 1976], was used because the forward model is somewhat nonlinear. The basic aim of OE is to minimize a cost function $C(\mathbf{x})$ given by

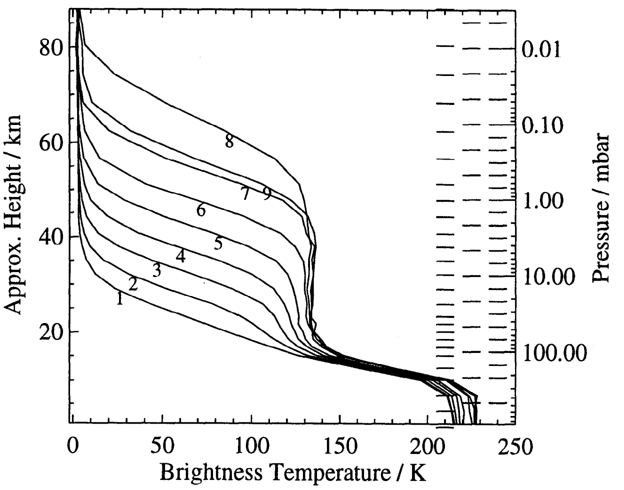

Figure 1. Radiances from channels 1-9 of Microwave Limb Sounder band 5. The data are for a single scan taken at 14.5°N, 89.5°E on August 26, 1992. Channels 10-15 are not shown but are similar to 1-6. The three sets of horizontal lines are, from left to right, the tangent pressures at which the measurements were made, the pressure grid used for versions 3 and 4 and the pressure grid used for the prototype described in this paper.

$$\begin{aligned} C(\mathbf{x}) &= (\mathbf{x}-\mathbf{x}_a)\mathbf{S}_a^{-1}(\mathbf{x}-\mathbf{x}_a) \\ &\quad + (\mathbf{y}-F(\mathbf{x}))\mathbf{S}_y^{-1}(\mathbf{y}-F(\mathbf{x})) \end{aligned} \tag{1}$$

We require an a priori value $\mathbf{x}_a$ for the state vector. The matrices $\mathbf{S}_y$ and $\mathbf{S}_a$ represent the covariances of $\mathbf{y}$ and $\mathbf{x}_a$, respectively. OE provides a formula (or in the nonlinear case an iterative algorithm) to calculate $\hat{\mathbf{x}}$, the value of $\mathbf{x}$ which minimizes $C(\mathbf{x})$, and its covariance matrix $\hat{\mathbf{S}}$.

As with version 4 the measurement vector $\mathbf{y}$ contained radiances from the 15 channels of MLS band 5; this band is centered on the 183.3 GHz line of water vapor. Figure 1 shows typical radiances from one scan. Note that the vertical coordinate used for MLS is log(pressure). The figures in this paper show "approximate height" as an alternative vertical coordinate. This coordinate is actually $(-16\text{ km}) \times (\log_{10}(\text{pressure/bars}))$, that is, pressure changes by a factor of 10 over 16 km of the "approximate height" coordinate. A complete scan always contains data from 26 different tangent altitudes so that $\mathbf{y}$ contains $15 \times 26 = 390$ elements. Although the layout of the channels is symmetrical about the band center, it can be seen from Figure 1 that there is a significant difference between channel 7 and channel 9 which are centered -2 MHz and +2 MHz from the line center, respectively. This is because the line is Doppler shifted by a combination of the Earth's rotation and the motion of the satellite. This effect is different on the ascending and descending sides of the orbit.

The function F is known as the forward model (FM). It models radiative transfer in the atmosphere and the characteristics of the instrument. The forward model code used in the prototype retrieval was developed along with the retrieval code at Edinburgh. Comparisons have been made with the Jet Propulsion Laboratory forward model used for version 4. Differences between the outputs of the two models are small compared to the experimental error if the two models use the same instrumental and spectroscopic parameters. The FM includes the Doppler shift explicitly, using a line-of-sight velocity supplied with the version 4 data. As input, the FM requires a temperature profile and a set of tangent pressures as well as a water vapor profile. We used the retrieved temperatures and tangent pressures from version 4; their uncertainties were incorporated into $\mathbf{S}_y$.

The measured radiances $\mathbf{y}$ contain a spectrally invariant offset or "baseline" of a few kelvins which varies slightly with altitude. One source of this offset is radiation emitted by the antenna. The antenna is hotter at the beginning and end of a UARS yaw cycle than it is for the rest of the cycle; this happens as a result of the changing angle between the Sun and the spacecraft. The baseline is consequently larger at these times. Yaw cycle dependences of the retrieved products are at least partly caused by this effect. The baseline must be estimated in order to get a good retrieved product. In versions 3 and 4 this was done by including it in the state vector and retrieving it along with the geophysical parameters. In the prototype a more conservative approach was taken. Above 45 km there is no signal from the atmosphere in channels 1 and 15 so the baseline may be estimated from these channels before performing the retrieval. Below 45 km we simply use the 45 km value. Estimated errors in the baseline are incorporated into $\mathbf{S}_y$; these errors are assumed to be the size of the channel 1 measurement error above 45 km and to increase below this level.

The a priori profile $\mathbf{x}_a$ is taken from a monthly zonal mean climatology composed of Stratospheric Aerosol and Gas Experiment (SAGE) 2 data in the lower stratosphere and Halogen Occultation Experiment (HALOE) (version 17) data in the upper stratosphere and mesosphere [*Pumphrey et al.*, 1998]. This climatology was also used for version 4 and is an improvement on the one used for version 3 in that it does not have extremely unrealistic values at 100 mbar and extends to a greater altitude. Throughout most of the stratosphere and mesosphere the retrieved product depends only very slightly on the a priori.

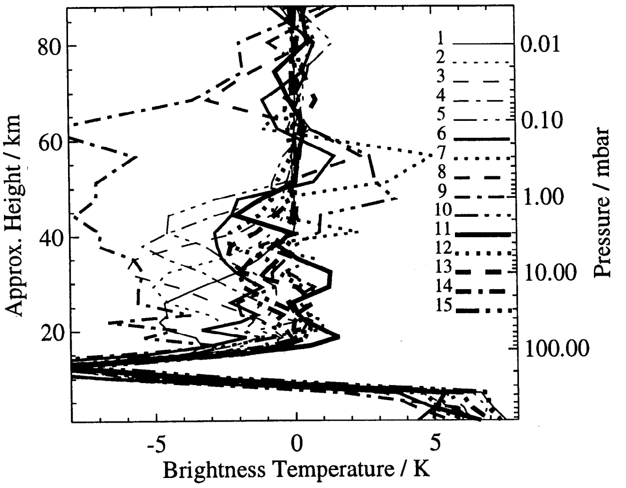

Figure 2. Residuals, that is, the difference between measured and recalculated radiances for the scan shown in Figure 1. Forward model parameters were those used for version 4. There is one line for each channel; the legend shows which channel is represented by which style of line.

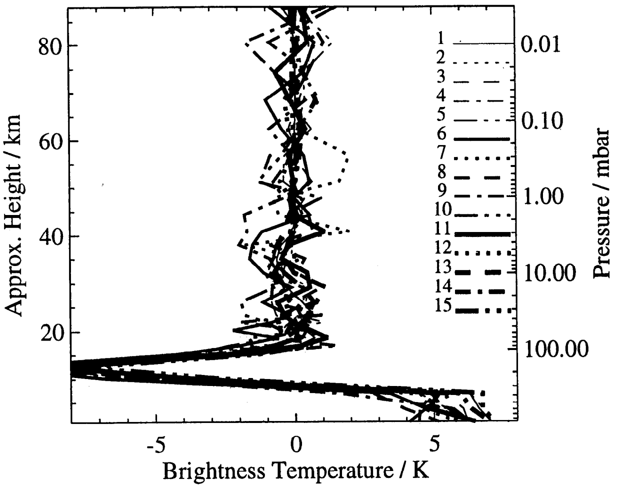

Figure 3. Residuals, that is, the difference between measured and recalculated radiances for the prototype. Details as for Figure 2.

The version 3 retrieval had serious closure problems, that is, the radiances re-calculated from the retrieved profiles did not match the measured radiances well [*Lahoz et al.*, 1996]. This implied that there were problems with the radiative transfer model. These problems were corrected for in a somewhat ad-hoc manner in both version 4 and the prototype described in this paper. In version 4, the instrument's sideband ratios were empirically adjusted in an attempt to improve closure. This was only partially successful because the retrieval is somewhat overdetermined; it simply is not possible to make $F(\mathbf{x})$ agree with $\mathbf{y}$ by adjusting only the water vapor and sideband ratios. In the prototype, two forward model parameters were adjusted for each channel before the retrievals were done; this seems to be a sufficient number of free parameters for a good fit to be possible. The parameters are (1) the sideband ratio and (2) the frequency offset of the channel from the band center. Figures 2 and 3 show the effect this procedure had on the closure of the retrieval. Clearly the forward modeling problems have been greatly alleviated, but we have to ask what justification there is for these adjustments. For the sideband ratios this is not a problem. These were measured as part of the prelaunch calibration process [*Jarnot et al.*, 1996] but for band 5 it proved very hard to obtain useful results. The measured radiances contain sufficient information to determine the water vapor and the sideband ratios, and it turns out that it is possible to make a better estimate of these quantities from the in-flight data than it was before launch (H. C. Pumphrey and S. Bühler, Instrumental and spectral parameters: their effect on and measurement by microwave limb sounding of the atmosphere, submitted to *Journal of Quantitative Spectroscopy and Radiative Transfer*,; hereinafter Pumphrey and Bühler, submitted manuscript, 1998). The channel frequency offsets, on the other hand, were measured very accurately before launch. By changing these in the forward model, we are not correcting for insufficient calibration, but for various physical effects which are not completely understood. One of these effects is that the 183.3 GHz line is pressure shifted as well as pressure broadened. In work done after the prototype described here was created, we have successfully retrieved values for the sideband ratios, as well as the pressure shift parameter, from zonally averaged radiances (Pumphrey and Bühler, submitted manuscript, 1998). The next official version, version 5, will use these corrected instrumental and spectral parameters instead of making arbitrary adjustments to filter locations, but the effect on the residuals and indeed on the retrieved product is similar.

Version 4 data were retrieved on every other UARS pressure level (... 10, 4.6, 2.2, 1 mbar ...); these levels are approximately 5 km apart. The new prototype was retrieved on every UARS surface (... 10, 6.8, 4.6, 3.2, 2.2, 1.5, 1 mbar ...) from 100 mbar up to 0.1 mbar; these levels are approximately 2.5 km apart. Above this, the version 4 grid is used as the instrument in its normal scan mode is only capable of a 5-7 km vertical resolution in the upper mesosphere. Figure 1 shows the pressure levels on which version 4 and the prototype were retrieved and also the tangent pressures for a typical limb scan; it is clear that the grid chosen for the prototype is better matched to the scan pattern than was the grid used for versions 3 and 4.

To quantify the vertical resolution somewhat, we calculate the averaging kernels [*Rodgers,* 1980] for a typical profile, these are shown in Figure 4. It is clear from Figure 4 that the vertical resolution in the stratosphere is indeed good enough to warrant the chosen grid. Note that the averaging kernel for 68 mbar is satisfactory in that it is reasonably narrow and is peaked at 68 mbar. The averaging kernel for 100 mbar not only is rather broad but also peaks at 68 mbar, not at 100 mbar. This is a clear indication that the 100 mbar data are of doubtful quality and probably consist to a large extent of the a priori. This suspicion is added to by the line in the figure showing the sum of the averaging kernels at each altitude. This sum should be approximately unity in regions where the retrieval is satisfactory – at 100 mbar it is approximately 0.4. We note that this is an equatorial profile and that the retrieval at 100 mbar is somewhat more successful at higher latitudes owing to the smaller optical depth of the atmosphere.

The vertical resolution in the mesosphere is poorer, largely because the scan pattern is coarser. The scan resolution is shown in the figure as a short-dashed line. Between 50 and 60 km the averaging kernel width seems to alternate between large and small values. This probably related to the fact that the scan pattern in this region is coarser than the retrieval grid. The kernel for a particular height will have a different shape if a scan level happens to be very close to that height than if this is not the case.

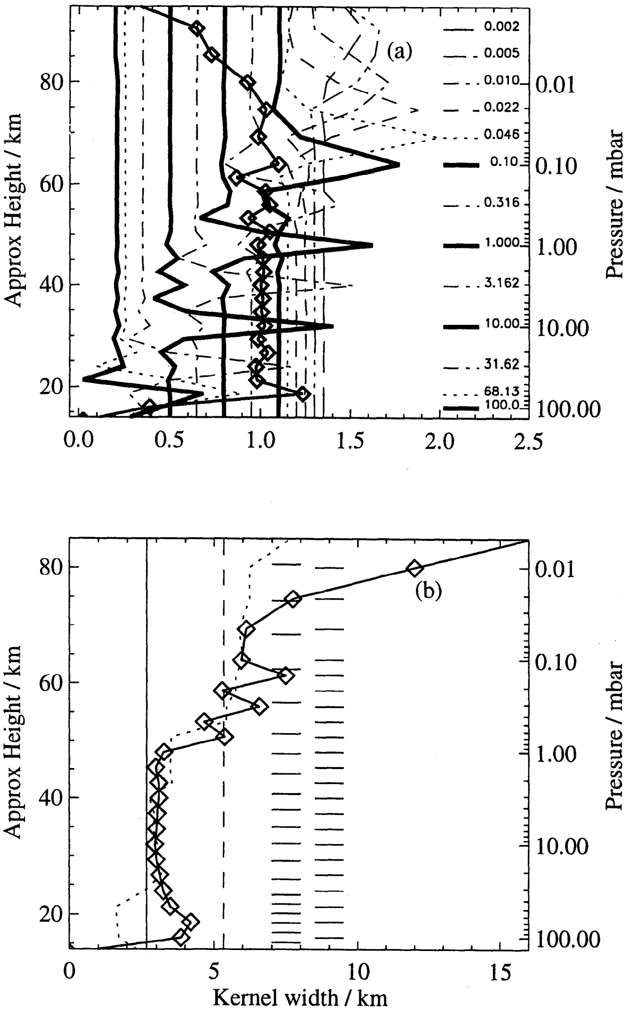

Figure 4. (a) Averaging kernels for some of the pressure levels on which water vapor is retrieved. The kernels are displaced to the right by an amount proportional to the altitude to which they refer to make the figure clearer. Kernels are not shown for all retrieval levels in order to reduce clutter. The line with diamonds is the sum of all the averaging kernels at each altitude. (b) Width of the averaging kernels as a function of altitude. The width is presented in the same "approximate height" units as the altitude. The two sets of horizontal lines indicate the tangent altitudes for this scan (left) and the retrieval grid (right). The short-dashed line is the distance between the closest two scan altitudes. All data are from the same scan as Figure 1.

For the purposes of identification, file naming, etc., the new prototype described in this paper is referred to within the MLS group as version 0104. The "01" is because this is the first such prototype version, the "04" because it is based on the version 4 temperature and pointing retrievals. This numbering convention is not an official, UARS project-approved MLS version number.

3. Comparison of Data With Other Measurements

In this section we compare the prototype version 0104 and the previous official version, version 4, to various other data sets. For each of these data sets the difference was taken between the non-MLS profile and the closest MLS profile for the same day. The two profiles are typically separated by less than 15° in longitude and 2° in latitude. The difference is averaged over a number of pairs of profiles to give a mean difference which gives an indication of the systematic bias between the two instruments; this is shown in the comparison figures as a solid line. We also average the square of the difference and take its square root to give a root-mean-square (RMS) difference which is shown in the comparison figures as a dotted line. This will be equal to the absolute value of the mean difference if all of the difference is systematic and greater if some of the difference is random. To aid this comparison where the mean difference is negative, the absolute mean difference is shown in the figures as a dashed line. The RMS difference should be of a similar size to the root-sum-square combined uncertainties of the two measurements, which is shown in the figures as a dot-dash line.

The general picture obtained by comparison with UARS HALOE, ground-based microwave data, and balloon-mounted frost point hygrometers is that the prototype is better than version 4 (which in turn is known to be better than version 3). Comparisons with the ATMOS instrument are less conclusive. It also emerges that the ascending-descending differences are much smaller in the prototype data than in version 4. It should be emphasized that these improvements come as a result of trying to improve the closure of the MLS retrieval not as a result of trying to make the MLS results more like those from other instruments.

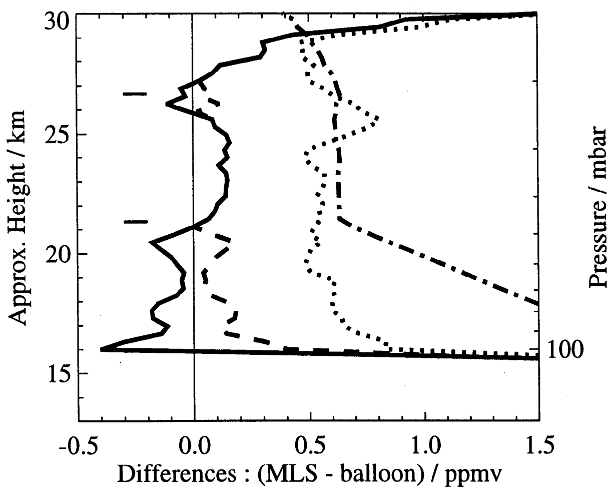

Figure 5. Mean difference (solid line) and the RMS difference (dotted line) between the balloons and MLS version 4 in parts per million by volume (ppmv). The dashed line is the absolute value of the mean difference and the dot-dash line is the mean MLS uncertainty as returned by the retrieval. Horizontal lines on the left show the MLS grid.

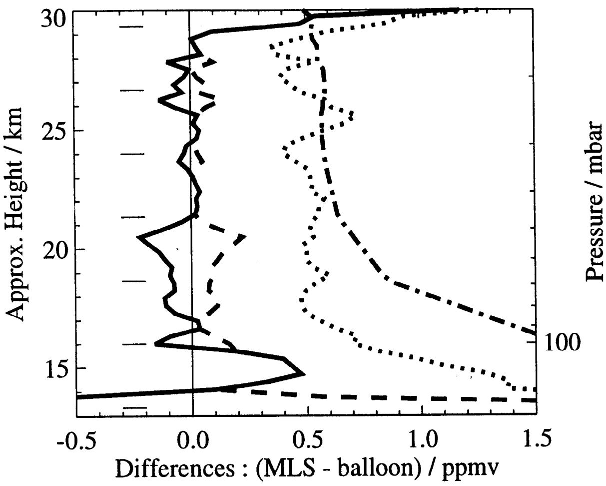

Figure 6. As Figure 5, but for the prototype, version 0104.

3.1. Comparison With Balloon Frost Point Hygrometer

There are 16 balloon-mounted frost-point hygrometer profiles available for which there are reasonably close MLS measurements. Figure 5 shows an average of the MLS-balloon differences for version 4. The short horizontal lines on the left show the levels at which the MLS data are retrieved. Between these levels, MLS mixing ratio is assumed to vary linearly in log(pressure). The agreement is good at 22 and 46 mbar. The RMS difference is similar to the error bars, or uncertainties, returned by the retrieval, and the mean difference is small compared to the RMS difference. Version 4 is not retrieved at 100 mbar and there are too few Balloon data at 10 mbar for a useful comparison to be made.

Figure 6 shows an average of the MLS-balloon differences for prototype version 0104. Agreement is as good or better than version 4. The improvement comes mainly from the fact that the prototype is retrieved on twice as many levels. There is better agreement at 100 mbar because the prototype is retrieved at this level and version 4 is not. The prototype at 100 mbar is dependent on the a priori to an extent which is normally considered unsatisfactory, however it is clearly managing to improve on the a priori to some extent.

3.2. Comparison With Ground-based Microwave (WVMS) Data

The Water Vapor Millimeter-Wave Spectrometer (WVMS) is a ground-based instrument which measures water vapor in the middle atmosphere. It measures thermally emitted microwave radiation in the 22 GHz region. Full details are given by *Nedoluha et al.* [1995], and a detailed comparison with other instruments is given by *Nedoluha et al.* [1997]. The latter paper and that of *Lahoz et al.* [1996] both show comparisons between WVMS and MLS version 3 data; both MLS version 4 and prototype version 0104 agree better with WVMS than does MLS version 3. During the time when MLS was measuring water vapor, WVMS spent some time at Table Mountain Observatory (TMO) in California and some

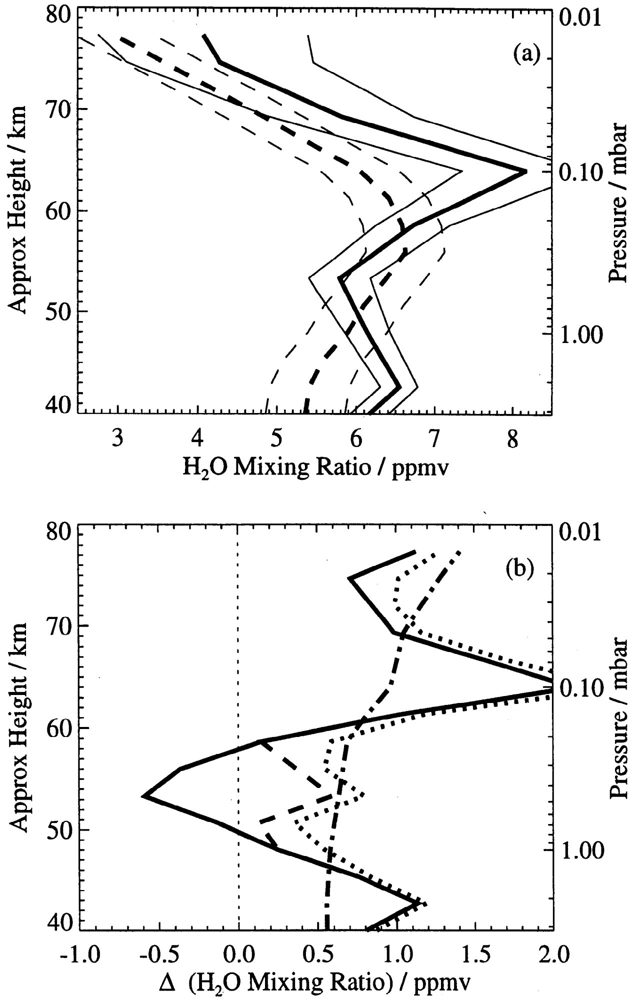

Figure 7. (a) Mean WVMS profile (dashed line) and mean coincident MLS version 4 profile (solid line) for January 9 to February 9, 1993. (b) Mean difference (solid line) and RMS difference (dotted line) between WVMS and MLS version 4. The dashed line is the absolute value of the mean difference. The dot-dash line is the root-sum-square of the mean MLS uncertainty as returned by the retrieval and the estimated error of WVMS, taken to be 0.5 ppmv.

at Lauder, New Zealand (45°S). WVMS profiles are usually available at 24-hour intervals; on some days no profile is available on account of weather conditions. In Figures 7a and 8a we show the mean profiles from MLS and WVMS for the period January 9 to February 9, 1993, when WVMS was at Lauder; the TMO data are not dissimilar. Figures 7b and 8b show the mean and RMS differences between MLS and WVMS. MLS version 4 shows clear systematic differences from WVMS which are not accounted for by the quoted error budgets of the two instruments. On the other hand, WVMS and the prototype agree to within their quoted uncertainties at most levels. The systematic component of the difference is a substantial proportion of the total difference, but the agreement is much better than for MLS versions 3 and 4. The most significant disagreement between the prototype and WVMS occurs at 0.2-0.3 mbar, where the MLS profiles show a notch. This feature probably has too small a vertical extent for WVMS to detect it.

3.3. Comparison With UARS HALOE

The HALOE instrument on UARS [*Russell et al.,* 1993] is a solar occultation instrument; it measures water vapor in the middle atmosphere by a very different technique from MLS. HALOE measures only 30 profiles per day: 15 sunrises near one latitude and 15 sunsets near another latitude. These latitudes drift gradually, so HALOE covers a reasonably wide range of latitudes during the course of a month or so. We use version 18 of the HALOE data.

Figures 9 and 10 show HALOE-MLS comparisons using HALOE measurements from a south-north sweep. Mean profiles are shown in Figures 9a and 10a and differences in Figures 9b and 10b. The agreement with version 4 is reasonable in that the RMS difference is less than the combined quoted uncertainties. However the quoted uncertainties on the HALOE data are rather large. Averaged over the whole sweep, the systematic differences are clear and change sign several times as over the altitude range shown. As with

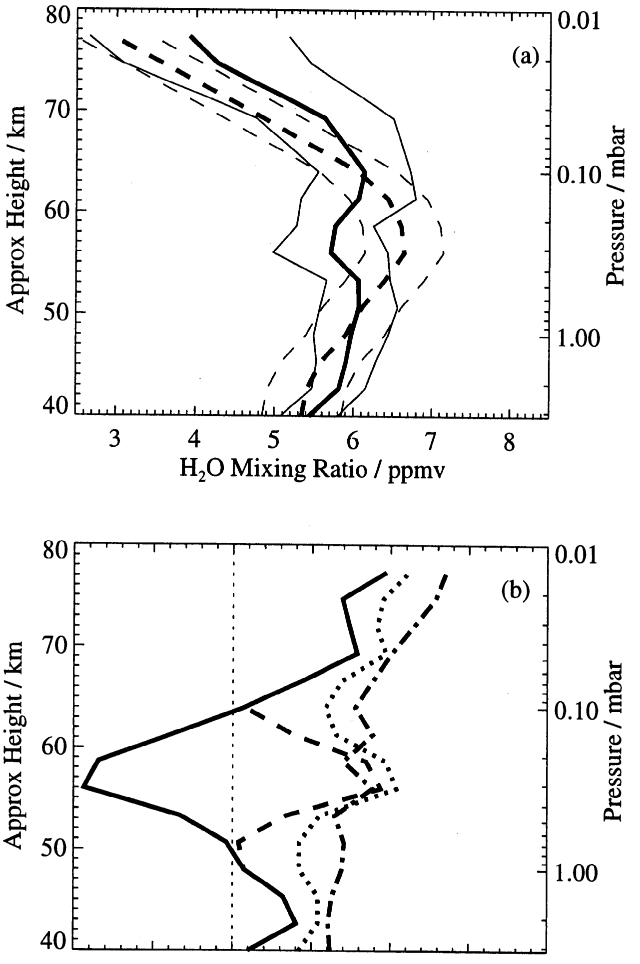

Figure 8. As Figure 7 but for the prototype version 0104 MLS data.

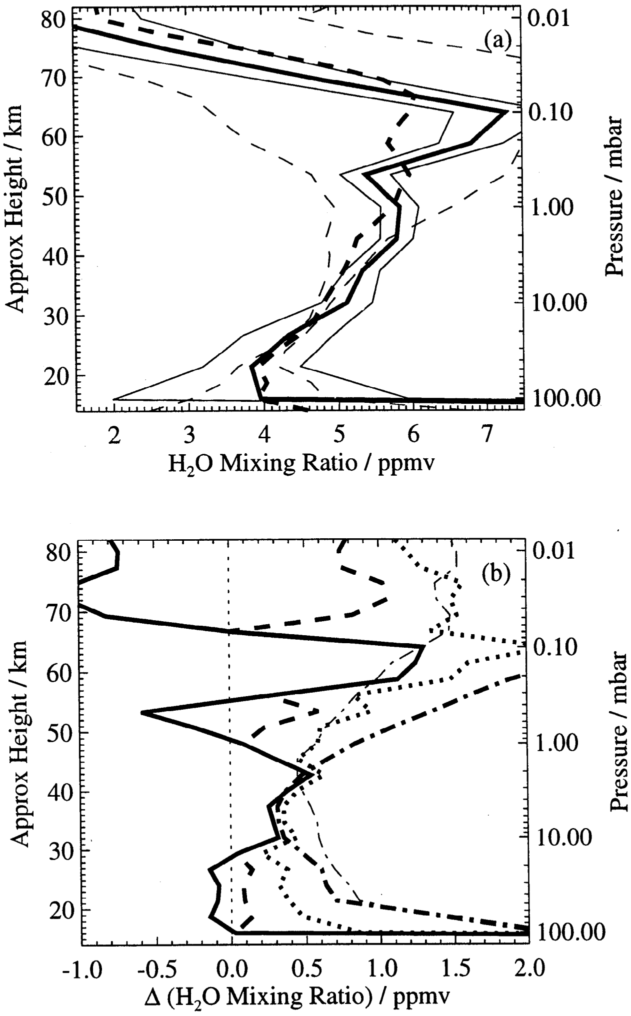

Figure 9. (a) Average HALOE (version 18) profile (dashed lines) and average coincident MLS version 4 profiles (solid lines) for the period October 29 to November 19, 1992. The bold lines denote the mean, and the thinner lines represent the typical uncertainty in a single profile. (b) Mean difference (solid line) and the RMS difference (dotted line) between HALOE and MLS. The dashed line is the absolute value of the mean difference and the dot-dash line is the root-sum-square of the mean MLS uncertainty and the mean HALOE uncertainty as returned by the retrievals. The thin dot dash line is the same as the thick one except that the standard deviation of the HALOE data is taken as an estimate of the single profile uncertainty instead of using the quoted estimate.

WVMS the systematic differences suggest that version 4 is too dry at 0.46 mbar and too wet at 0.22 mbar and 0.1 mbar. The MLS data are taken only from the descending leg of the orbit; the systematic errors are somewhat different for the ascending leg. The agreement between HALOE and the prototype is better, with the systematic difference being about half of the RMS difference at most heights. Also, the systematic differences are similar for the ascending and descending legs of the orbit. The prototype MLS mixing ratios are uniformly lower than the HALOE mixing ratios.

The double peak in the HALOE data at 52 and 64 km is a feature of great interest in the understanding of OH (hydroxyl) chemistry in the mesosphere [*Siskind et al.,* 1998; *Summers et al.* 1997]. This feature seems to be present in the prototype MLS data shown in Figure 10, but to a much smaller extent; its presence has already been noted in this paper in connection with Figure 8. In MLS version 4 this feature is swamped by the large systematic errors described above. It should be noted that if the feature is real, the limited vertical resolution of MLS will prevent the upper peak from being as clearly resolved as it is in the HALOE data.

In order to clarify this issue, a test was carried out. A mean HALOE profile was generated for UARS days 426-430 (November 10–14, 1992), a time when the double peak was prominent. Calculated MLS radiances were generated using this profile as input to the FM; these were then used as input for the retrieval software. The resulting retrieved profile is essentially the HALOE profile smoothed by the MLS averaging kernels, that is, it is what MLS is expected to see if the true profile were the same as the HALOE profile. It is shown in Figure 11 along with the original average HALOE profile. Clearly, there is little difference between

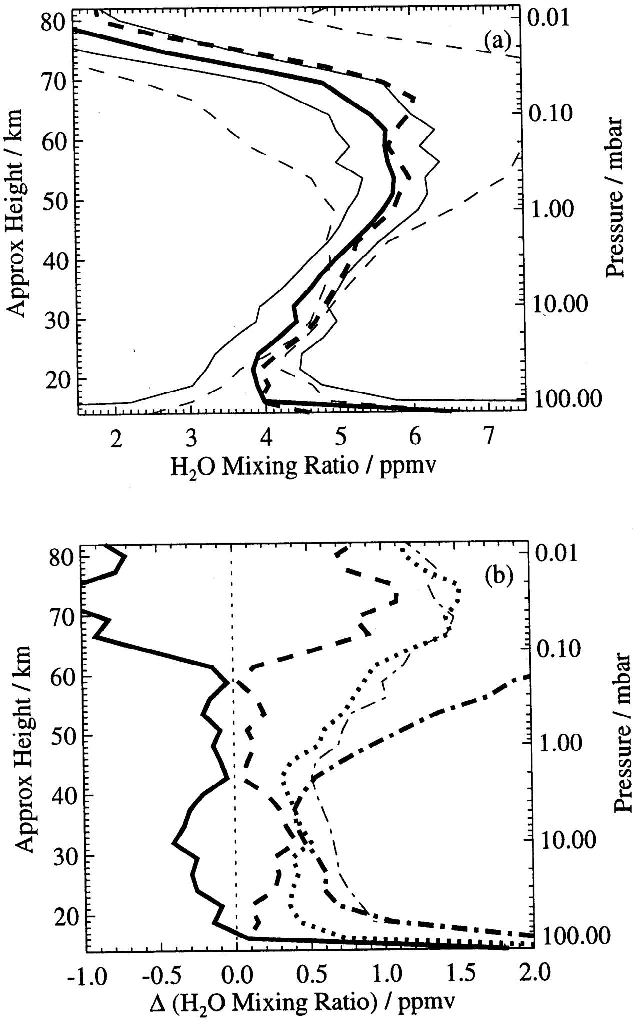

Figure 10. As Figure 9 but for the prototype MLS data.

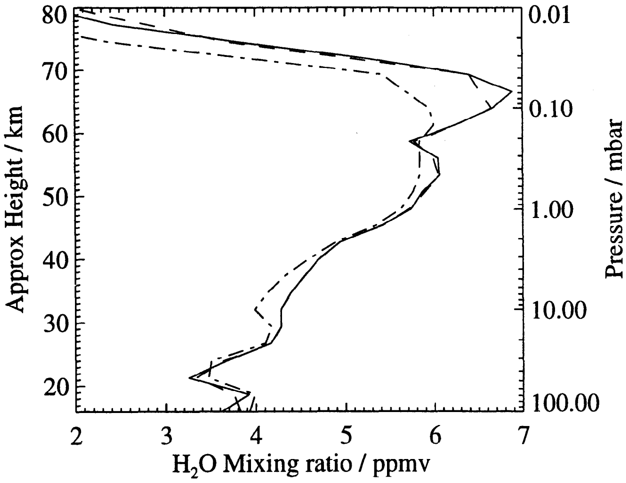

Figure 11. Test to see if HALOE double peak is consistent with MLS observations. Solid line denotes HALOE, dashed line denotes test retrieval, that is, what MLS is expected to produce if HALOE were correct, and dot-dash line denotes version 0104 average. Clearly, there is a systematic difference between MLS and HALOE in the mesosphere which is not simply caused by the limited resolution of MLS.

the two except at 0.068 mbar. The HALOE profile was interpolated onto the version 0104 grid (which does not include this level) before it could be used as input to the FM, and this accounts for most of the difference. The figure also shows the mean MLS version 0104 profile for this period. The systematic difference between HALOE and MLS version 0104 in the mesosphere is clearly not simply one of vertical resolution and must be caused by other effects. One such effect which we can eliminate is the possibility that the structure is present in the retrieved data solely because a similar structure is present in the a priori. A retrieval of a single day's data was carried out using a very simple a priori consisting of a single profile with no double peak. The retrieved product from this test had a double peak similar to that seen in version 104. Since both instruments show a double-layer structure, we conclude that this structure is likely to be a real feature of the atmosphere. There remains a large inconsistency of 0.8 ppmv in the magnitude of the upper peak between the two instruments.

As an additional check on this MLS-HALOE inconsistency, we show in Figure 12 the difference between radiances calculated from the HALOE profile and those measured by MLS. The difference is largest in the upper mesosphere, from which we conclude that either the HALOE profile is wetter than the true one in this region and/or that the MLS forward model has systematic errors in this altitude range.

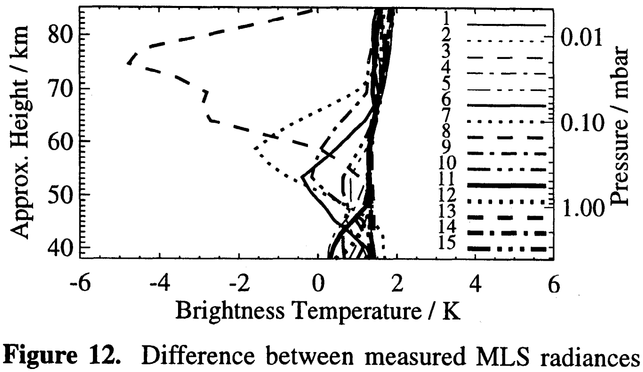

Figure 12. Difference between measured MLS radiances and radiances calculated from the HALOE profile. This difference is largest in the 60-80 km altitude range and in the channels 7, 8, and 9, the channels closest to the line center. This suggests that the HALOE profile is too wet and/or that the MLS FM has deficiencies in this range. Note that the noise on a single measurement in the line center channels is approximately 1 K. The baseline for this scan is about 1.5 K. The different line styles represent the 15 channels of MLS band 5, as in Figures 2 and 3.

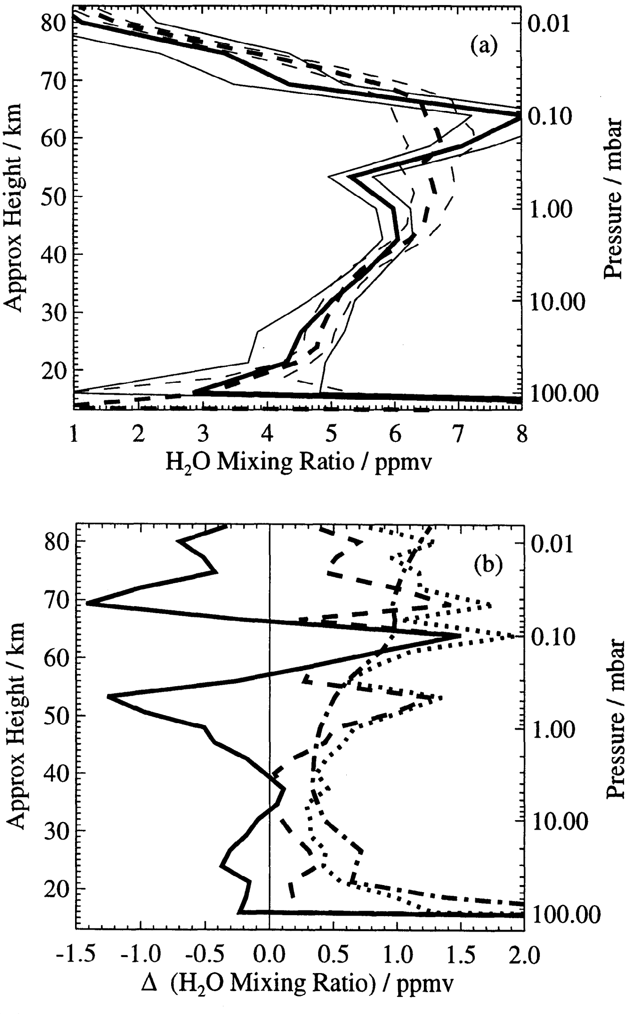

Figure 13. (a) Average ATMOS profile (dashed lines) and average coincident MLS version 4 profile (solid lines) for the period of the Atlas 1 mission (March 25 to April 1, 1992). The bold lines denote the mean, and the thinner lines represent the typical uncertainty in a single profile. (b) Mean difference (solid line) and RMS difference (dotted line) between ATMOS and MLS. The dashed line is the absolute value of the mean difference and the dot-dash line is the root-sum-square of the mean MLS uncertainty and the mean ATMOS uncertainty as returned by the retrievals.

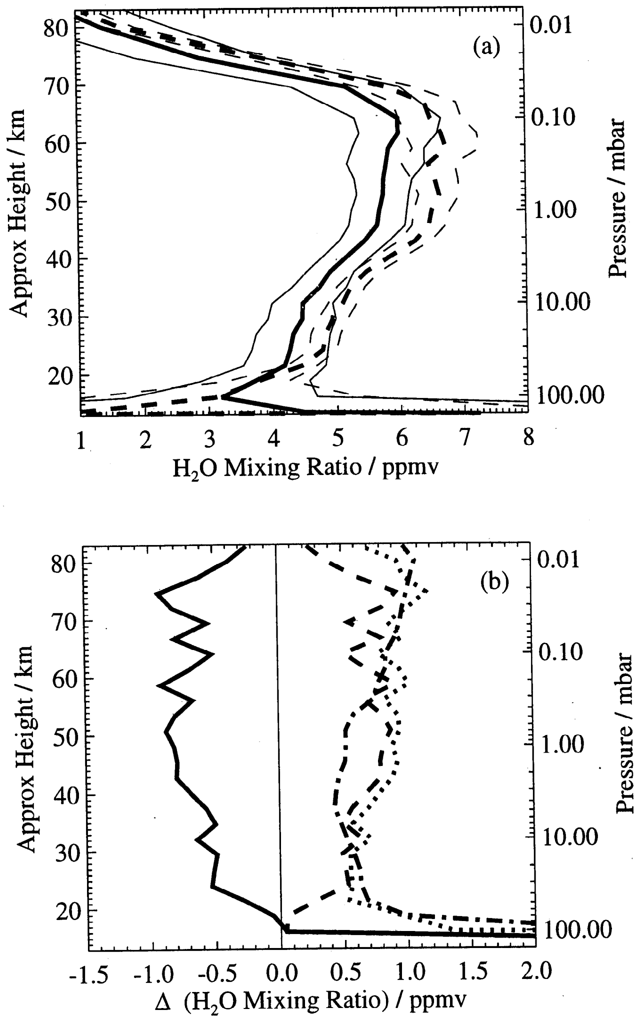

Figure 14. As for Figure 13 but for prototype MLS data.

3.4. Comparison With ATMOS

The ATMOS instrument [*Gunson et al.*, 1990, 1996] measures a number of trace species by solar occultation. ATMOS was flown on the Space Shuttle twice during the period when MLS was making measurements of water vapor. We show in Figures 13 and 14 a comparison between MLS and ATMOS using all the ATMOS sunset measurements taken during the Atlas 1 Space Shuttle mission and the coincident MLS profiles. The format of the figures is the same as for Figures 9 and 10.

Version 4 agrees well with ATMOS in the lower and middle stratosphere. Above 45 km the MLS-ATMOS difference is large and oscillatory, as it was with HALOE. The agreement between the prototype and ATMOS is a little less satisfactory than with HALOE in that MLS is drier than ATMOS by about twice the amount. Furthermore, the RMS difference is not much larger than the absolute difference, indicating that most of the MLS-ATMOS difference is systematic. However, it is an offset which changes little with altitude.

It seems likely on the basis of the four comparisons shown above that the prototype MLS H_2O data set has a small dry bias, between 0.0 and 0.4 ppmv, in the lower stratosphere and a dry bias of between 0.2 and 0.7 ppmv in the upper stratosphere. However this bias changes quite slowly with altitude, a great improvement on versions 3 and 4.

4. Examination of the Data

In this section we display the prototype data set and examine some of the new features which appear in it. Where possible, we show version 4 as well, in order to bring out the differences between the two data sets. We note that in addition to the differences examined here, *Manney et al.* [1998] have shown that the 4-day wave in the polar upper stratosphere is more clearly visible in prototype version 0104 than it is in version 4. Figure 15 shows zonal means of the two versions. MLS either observes from 80°S to 34°N or from 34°S to 80°N; to show the full latitude range of the instrument, data south of the equator are from July 12, 1992 while data north of the equator are from July 19, 1992. The quality of the retrieval is assessed by taking the ratio of retrieved uncertainties and the a priori errors; we consider the retrieval to be useful if this ratio is less than 0.5. The thick unshaded contour marks where half of the retrievals in a latitude bin pass this test, the thin dotted contours either side of it are 10% and 90% pass rates. (Profiles where the retrieval failed completely are rejected before the zonal mean is taken.)

There are several clear differences; in particular, the prototype is free of the unusually high values at 0.1 mbar which are present in version 4. Note also that the prototype has usable data at lower altitudes. The double-peak structure seen in Figure 8 is present in the data but is not visible in the figure as the dip between the peaks is no bigger than the contour spacing.

Figure 16 shows a time series of MLS water vapor in the equatorial lower stratosphere with the time mean subtracted to bring out the seasonal cycles. Note the bands of dry and wet air which rise from the tropopause. These are thought to be the result of an annual cycle in temperature (and hence in saturation mixing ratio) at the tropical tropopause. This effect has been dubbed the "Tape recorder" [*Mote et al.*, 1996]. Note that the tape recorder signal is a great deal clearer in the prototype, mostly because the prototype is retrieved on every UARS level. Note also that both versions have artifacts which are due to the UARS yaw cycle, as discussed above, and due to the a priori being based on calendar months. To clarify which is which, the yaw days are marked with open bars and the calendar month boundaries are marked with solid bars. Both of these effects are less severe in the prototype than they are in version 4, implying that the prototype data are less affected by the a priori and by the yaw cycle dependence of the antenna temperature.

Because of the spike at 0.1 mbar, the MLS team has recommended that version 4 H_2O not be used at altitudes above 0.22 mbar. Since this spike is not present in prototype version 0104, we look at a time series of MLS H_2O in the upper mesosphere; this is shown in Figure 17. A pressure of 0.0046 mbar is chosen, as this is the highest altitude at which the retrieved product is not excessively contaminated with the a priori. The calendar month boundaries are marked

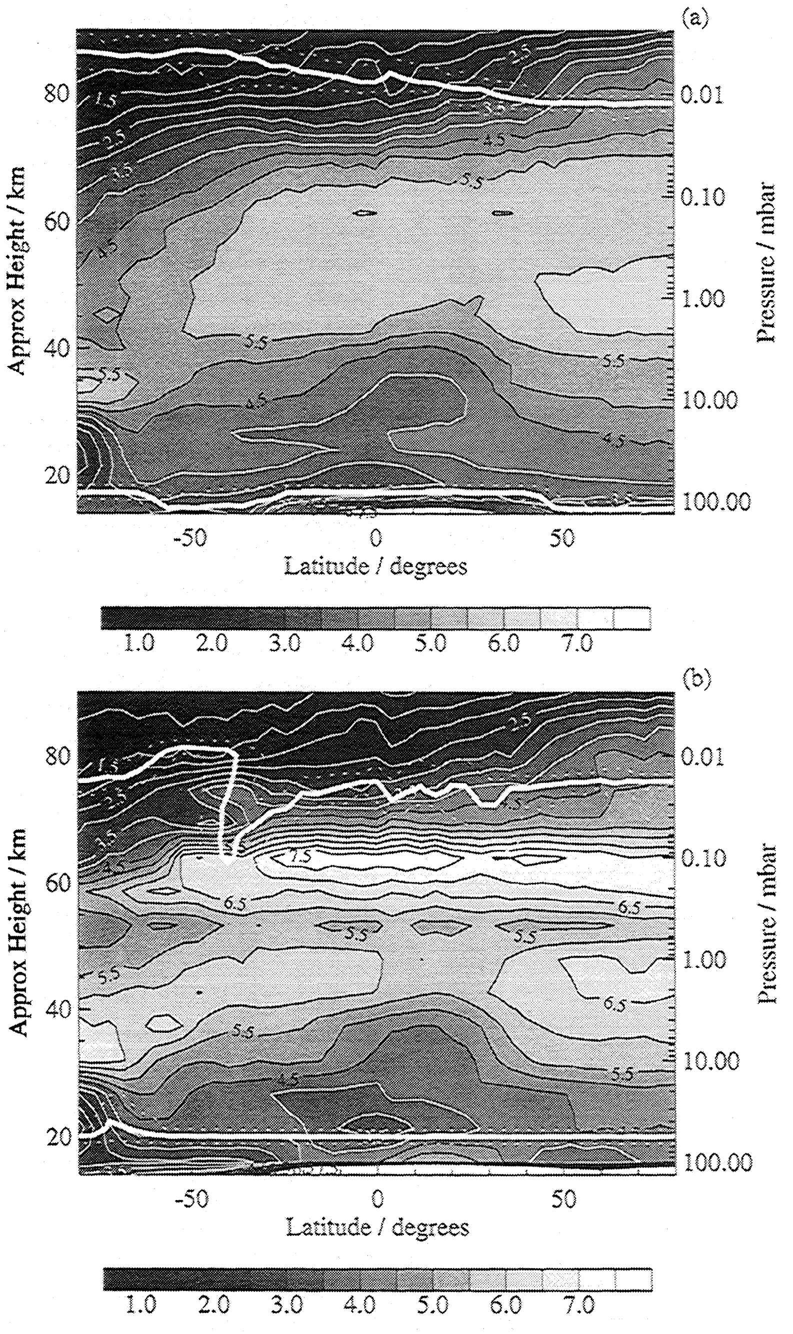

Figure 15. (a) Zonal mean of MLS (prototype version 0104) water vapor in mid-July 1992. (b) As Figure 15a but for MLS (official) version 4 data. See text for further details.

with open bars; sudden changes at these times are caused by the a priori. This problem is worst near the summer poles, consistent with the retrieval quality contour shown in Figure 15. The main feature to be seen is the large annual cycle at the poles, where a large amount of wet air is raised to this altitude during the polar summer. This wet air appears to be transported from summer pole to winter pole, giving a semiannual cycle at the equator and a combination of annual and semiannual cycles at other latitudes. Interestingly, version 4 and prototype version 0104 are very similar at this altitude, so whatever the problem was that affected version 4 at 0.1 mbar, its influence does not extend as far upward as was feared.

One of the known artifacts in version 4 H_2O is a difference between the ascending and descending legs of the orbit. This is a true ascending-descending difference, not a day-night difference and is therefore probably a systematic error. It is thought to be the result of an interaction between the Doppler shift of the line and the various systematic errors which were corrected for in the prototype by adjusting

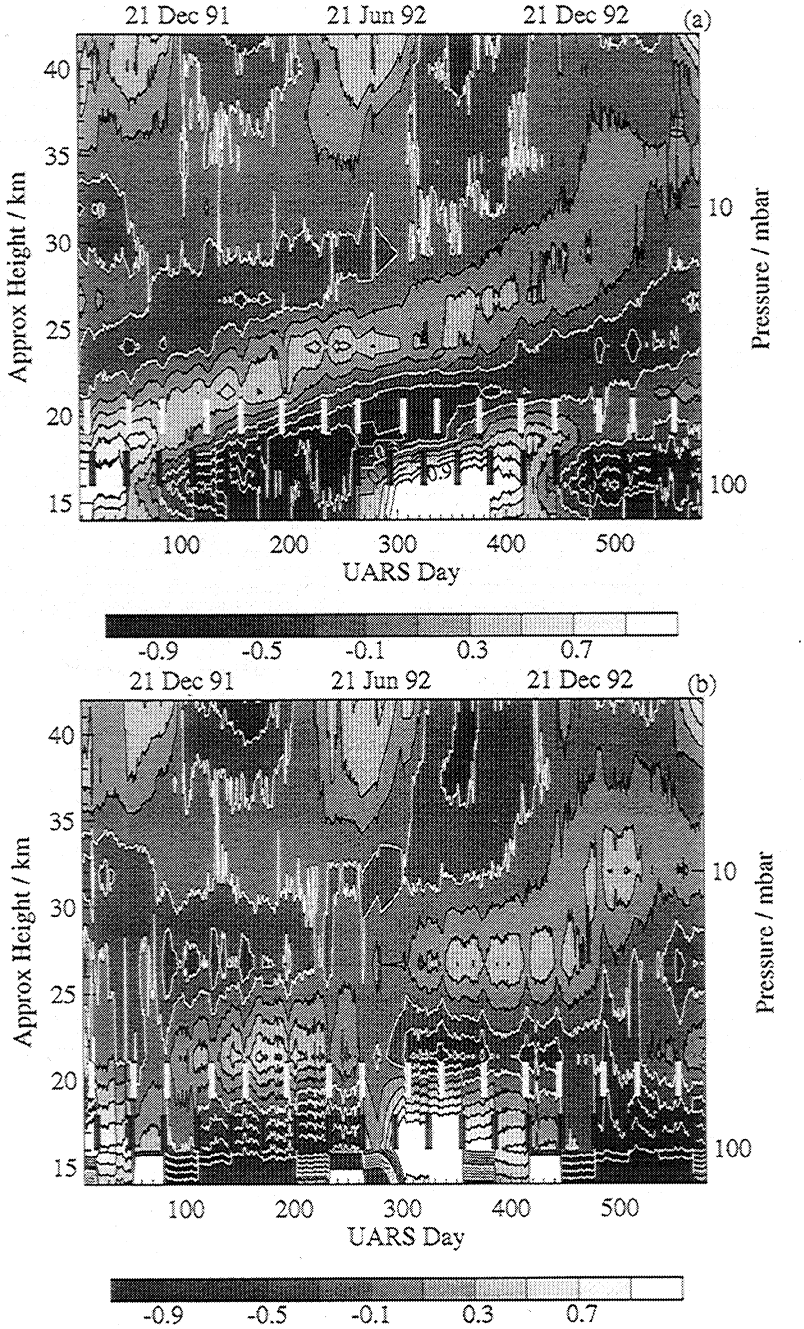

Figure 16. (a) A time series of MLS water vapor (version 0104) in ppmv at the equator; the time mean has been subtracted to bring out the seasonal cycles. The open bars mark UARS yaws, the solid ones are where the calendar month changes. (b) Same as Figure 16a, but for MLS version 4.

the channel frequencies. Figure 18 shows an example for March 19, 1992.

The prototype data have very small ascending-descending differences; in particular, the large differences seen between 1 and 0.1 mbar in version 4 are absent. There is, however, a feature at 0.01 mbar (about 80 km) which remains. The cause of this feature is not known; it may be a real physical effect, caused, perhaps, by the diurnal tide.

5. Conclusions

The prototype MLS water vapor data discussed in this paper, version 0104, are an improvement on the water vapor data in MLS version 4. They have better vertical resolution in the stratosphere and an improved forward model has reduced systematic errors, particularly in the mesosphere. As a result, these new data agree better with the available cor-

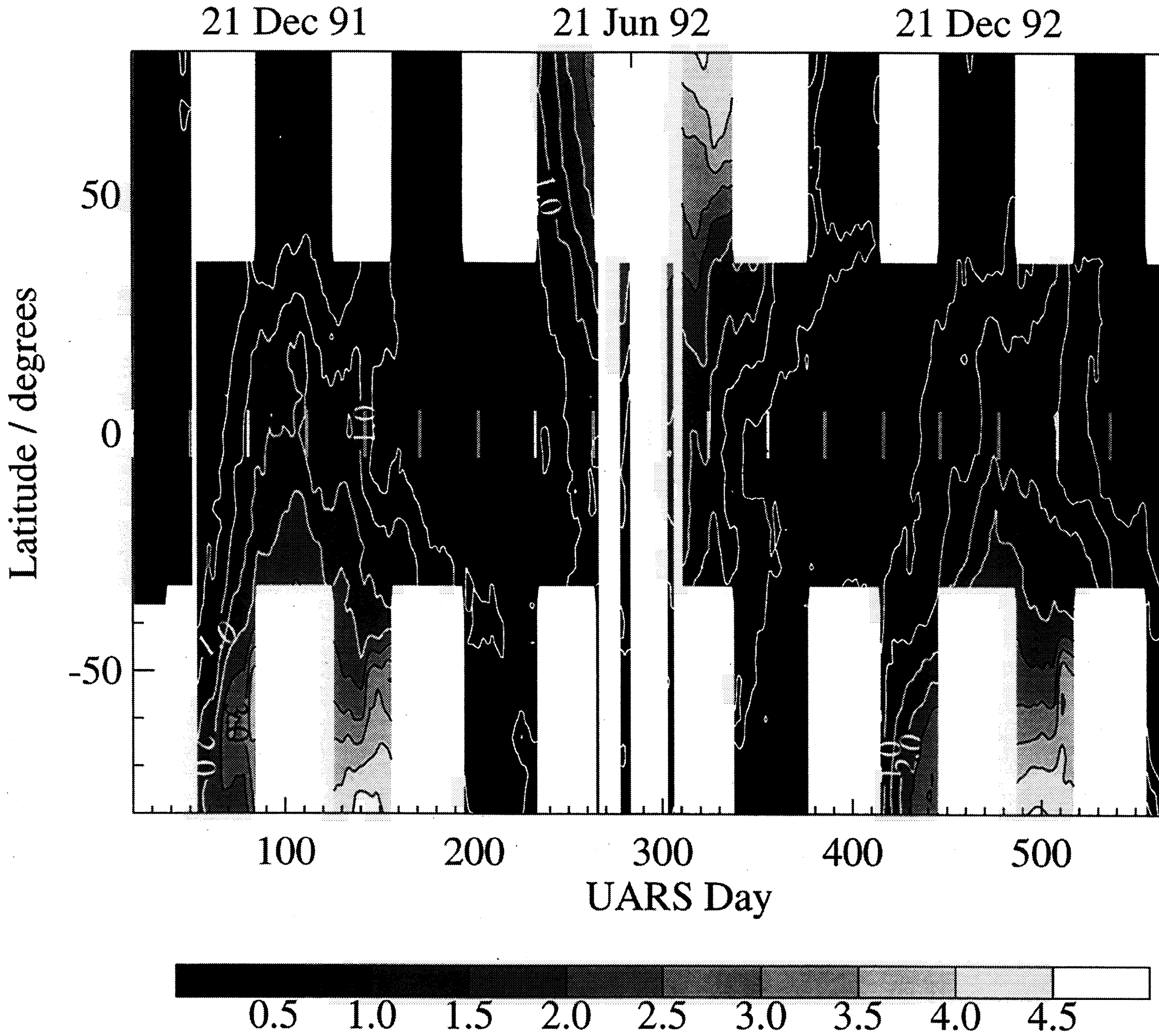

Figure 17. Time series of MLS water vapor (prototype version 0104) in ppmv at 0.0046 mbar (approximately 83 km). The gaps poleward of 34° are a result of the UARS yaw cycle. Other gaps, particularly those around day 300, are the result of operational problems.

relative measurements than did earlier versions. Specifically, the following improvements are noted:

1. The version 0104 data agree well with balloon-mounted frost point hygrometers between 100 mbar and 3 mbar.
2. The version 0104 data agree as well or better with WVMS than did earlier versions of MLS water vapor.
3. The version 0104 data agree as well or better with UARS HALOE than did earlier versions of MLS water vapor, between 100 mbar and 0.1 mbar. The improvement is most noticeable in the lower mesosphere. The new data are drier than HALOE by 0.1 to 0.4 ppmv over this altitude range. The double peak structure seen in HALOE data is present but the upper of the two peaks is much less prominent than it is in HALOE version 18. Above 0.1 mbar, MLS versions 4 and 0104 are both 1 ppmv drier than HALOE.
4. The version 0104 data agree acceptably with ATMOS between 100 mbar and 0.01 mbar. Between 30 mbar and 0.02 mbar version 0104 is drier by 0.5 to 0.7 ppmv. The version 4 values were closer to those of ATMOS in the stratosphere than the version 0104 values are. However, the variation with altitude in version 0104 resembles that of ATMOS more closely than does version 4.

Several of the problems in version 4 are cured in the prototype or are less severe; the most notable are the yaw cycle dependence and the ascending-descending differences. The combination of the improvements described above mean that the new data allow us to see more clearly several atmospheric phenomena. These include (1) the annual cycle of water vapor in the upper mesosphere, (2) the tape recorder effect in the equatorial lower stratosphere, and (3) the 4-day wave in the polar upper stratosphere.

MLS version 5 is in preparation at the time of writing, and the H_2O product will contain all the improvements seen in the prototype described here and several more. In particular,

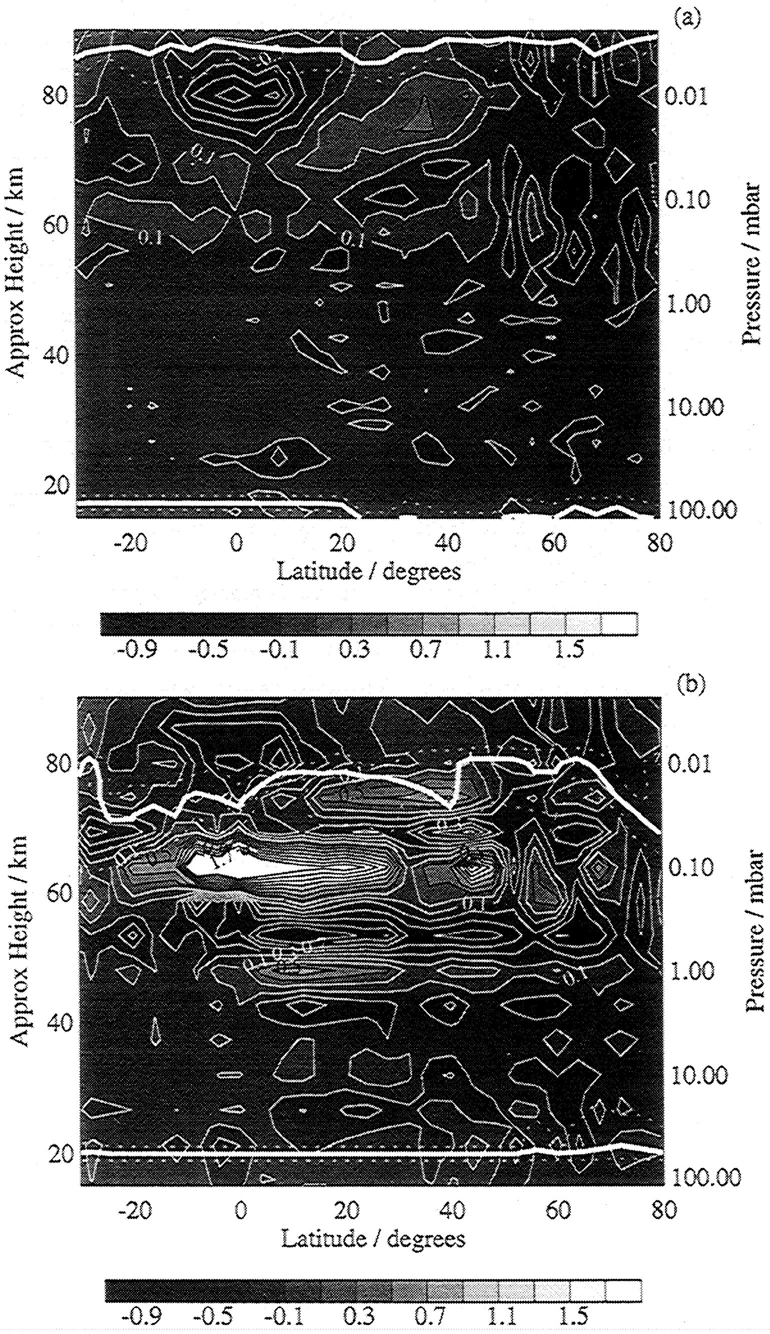

Figure 18. (a) Ascending - descending zonal mean for the prototype. (b) Same as Figure 18a, but for version 4. Data are for March 19, 1992.

improved temperature and pointing retrievals should mean that the H_2O retrieval in the mesosphere relies less on the a priori.

Acknowledgments. Thanks are due to the rest of the MLS team, in particular to Joe Waters, Bob Harwood, and Gloria Manney, who read the paper before submission and made many helpful suggestions. Thanks are also due to the HALOE team and to all the groups who supplied correlative data to the UARS project, in particular Gerald Nedoluha and Sam Oltmans, and to the ATMOS team. The paper was much improved by the comments of two anonymous reviewers. This work was supported by NERC, the U. K. Natural Environment Research Council, under grant number GR3/10111.

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(Received May 7, 1998; revised November 19, 1998;
accepted November 27, 1998.)