

## Validation of UARS Microwave Limb Sounder ozone measurements

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**Abstract.** This paper describes the validation of ozone data from the Upper Atmosphere Research Satellite (UARS) Microwave Limb Sounder (MLS). The MLS ozone retrievals are obtained from the calibrated microwave radiances (emission spectra) in two separate bands, at frequencies near 205 and 183 GHz. Analyses described here focus on the MLS Version 3 data (the first set of files made publicly available). We describe results of simulations performed to assess the quality of the retrieval algorithms, in terms of both mixing ratio and radiance closure. From actual MLS observations, the 205-GHz ozone retrievals give better closure (smaller radiance residuals) than that from the 183-GHz measurements and should be considered more accurate from the calibration aspects. However, the 183-GHz data are less noise limited in the mesosphere and can provide the most useful scientific results in that region. We compare the retrieved 205-GHz ozone profiles in the middle-to lower stratosphere to ozonesonde measurements at a wide range of latitudes and seasons. Ground-based lidar data from Table Mountain, California, provide a good reference for comparisons at higher altitudes. Based on these analyses, comparisons with balloon-borne measurements and others, as well as a detailed budget of estimated uncertainties, MLS results appear to be generally of high quality, with some biases worth mentioning. Results for the lowermost stratosphere ( $\sim 50$  to 100 hPa) are still in need of improvement. A set of estimated precision and accuracy values is derived for the MLS ozone data sets. We also comment on recent updates in the retrieval algorithms and their impact on ozone values.

### 1. Introduction

The Microwave Limb Sounder (MLS) aboard the Upper Atmosphere Research Satellite (UARS) has been performing emission measurements of the upper atmosphere on a global scale, day and night, since late September 1991. Descriptions and analyses of these and other UARS observations have been described in a variety of articles; in particular, special issues dealing

with UARS results can be found in the *Geophysical Research Letters*, volume 20 (12), 1993, and the *Journal of Atmospheric Science*, volume 51 (20), 1994.

This paper addresses the quality of MLS ozone data, their expected uncertainties (both random and systematic) as well as their demonstrated accuracy, based on comparisons with other data sets. This information should be of use to those attempting to use MLS ozone data, whether for comparison with other data sets, for absolute values to be used, for example, in radiative calculations, or for temporal and spatial variations, where precision matters more than accuracy. Since MLS ozone measurements are made from two independent radiometers (near frequencies of 205 GHz and 183 GHz), we discuss the quality of both of these data sets. However, we focus on the more accurate 205-GHz stratospheric results, at least in the intercomparisons with other data sets; these comparisons are weighted toward the middle and lower stratosphere, primarily because of the availability of data sets. Additional analyses of the 183-GHz ozone data in the mesosphere (where the measurement sensitivity is better than for 205 GHz) are presented by *Ricaud et al.* [this issue], in relation to models and ground-based measurements. Several validation work-

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shops have been held among UARS investigators since the launch of UARS, and the evolving results from those workshops have been documented [e.g., *Grose and Gille*, 1996]. Some validation of the zonal mean ozone values from MLS has already been provided in comparisons with Total Ozone Mapping Spectrometer (TOMS) total column data [*Froidevaux et al.*, 1994], where spatial and temporal variations are generally in good agreement. This includes, for example, the observed development of the ozone hole over Antarctica during southern winter and spring [see also *Manney et al.*, 1993; *Waters et al.*, 1993]. Another, less direct type of validation exists in the form of observed ozone variations or waves [e.g., *Canziani et al.*, 1994; *Elson et al.*, 1994; *Ray et al.*, 1994], to the extent that such variations can be understood, modeled, or “duplicated” in other data sets (current or past).

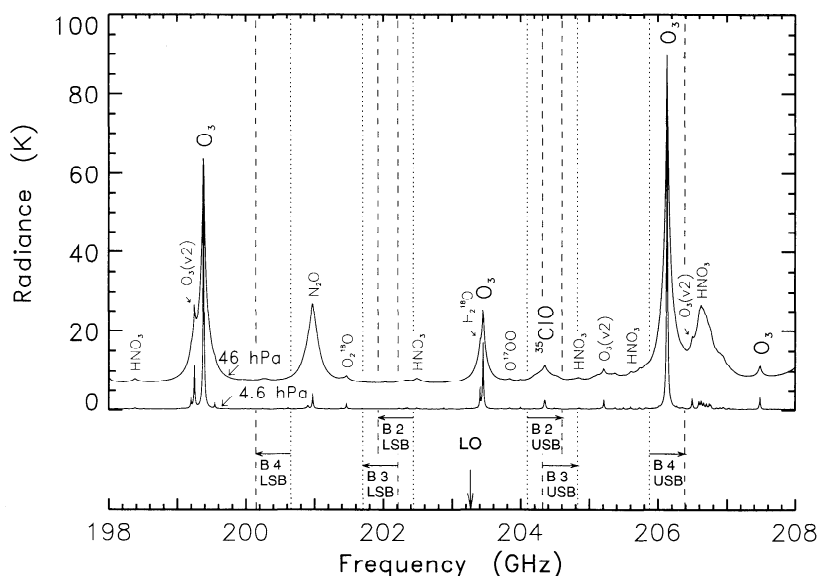
In this special issue on validation of UARS data, we describe in more detail certain aspects of the MLS ozone measurements (section 2), data processing and retrieval specifics (section 3 and Appendix), radiances and closure for both simulated data sets and actual data (section 4), estimated uncertainties based on expected sources of error (section 5), and comparison results (section 6). The comparisons here focus on non-UARS data sets, because for ozone at least, there exists a large amount of accurate correlative data. We comment only briefly here on other existing satellite data sets (see section 6); note that a significant source of validation for MLS ozone can be found in the work of *Cunnold et al.* [this issue (a)] [see also *Grose and Gille*, 1996], where statistical comparisons are made with coincident ozone profiles from the Stratospheric Aerosol and Gas Experiment (SAGE) II ozone data; this work helps to extend the analysis and validation of MLS 205-GHz ozone data into the stratopause region (and points out some systematic effects). Also, comparisons of UARS ozone measurements to each other and to other data sets can be found in the works of *Grose and Gille* [1996] and *Cunnold et al.* [this issue (b)]. We provide a summary of accuracy and single-profile precision values (see section 7) for the MLS Version 3 ozone data sets currently available. Updated results and plans for continuing improvements are described in section 8, before the concluding summary. We note that this special issue of the *Journal of Geophysical Research* contains validation papers for other atmospheric parameters from MLS, namely, tangent pressure and temperature [*Fishbein et al.*, this issue], chlorine monoxide [*Waters et al.*, this issue], and water vapor [*Lahoz et al.*, this issue]. In addition, *Jarnot et al.* [this issue] discuss the calibration of MLS radiances, a topic of much relevance to the validation of atmospheric parameters. Furthermore, a detailed description of the forward model used to calculate radiances which are tabulated and used as part of the retrieval process is forthcoming (W.G. Read et al., manuscript in preparation, 1996).

## 2. Measurements

UARS MLS measurements are obtained from observations of millimeter-wavelength thermal emission as

the instrument field of view (FOV) is vertically scanned through the atmospheric limb. A general description of microwave limb sounding and its features is given by *Waters* [1989, 1993], and the UARS MLS instrument is described by *Barath et al.* [1993].

Each of the 3 MLS radiometers (named “63-GHz,” “205-GHz,” and “183-GHz” radiometers because of the frequency near which they operate) receives emission, simultaneously, in a set of filter banks, each spanning 510 MHz in frequency space with 15 contiguous channels of varying width [see *Barath et al.*, 1993; *Jarnot et al.*, this issue]. The 63-GHz radiometer measurements (MLS band 1) provide tangent pressure and temperature information from O<sub>2</sub> emission spectra, the 205-GHz radiometer provides chlorine monoxide (ClO) (bands 2 and 3) and ozone (band 4), while the 183-GHz radiometer measures emission lines of water vapor (band 5) and ozone (band 6). In this paper we will commonly refer to the 205- and 183-GHz ozone data, following the above radiometer designation. The ozone lines are centered at 206.13205 GHz (1.45 mm wavelength) and 184.37782 GHz (1.63 mm wavelength), as listed by *Pickett et al.* [1992]. This spectral data catalogue and the references therein are the basis for the spectroscopic calculations used to model the ozone emission, along with the line width measurement by *Oh and Cohen* [1992]. The MLS instrument uses double-sideband heterodyne radiometers: signals from two sidebands, equally spaced about the local oscillator frequency, are combined (with slightly unequal weights) into a single measurement. The weights, or sideband ratios, are measured for each channel as part of prelaunch instrument calibration [see *Jarnot et al.*, this issue]. The primary sideband measures an atmospheric species of interest; the other is referred to as the image sideband. Figure 1 shows calculated radiances in the spectral domain covered by the 205-GHz radiometer, where ozone and ClO emission are the primary MLS targets, for typical upper and lower-stratospheric signals. Both primary and image sidebands are shown in Figure 1, for the MLS bands 2, 3, and 4 mentioned above. Useful information on other species that emit in this region has also been obtained; this includes SO<sub>2</sub> from the Mount Pinatubo eruption [*Read et al.*, 1993], HNO<sub>3</sub> [*Santee et al.*, 1995], and tropospheric H<sub>2</sub>O [*Read et al.*, 1995]. Other contributions include emission from the wing of a N<sub>2</sub>O line outside the target band pass, which becomes significant only in the lowermost stratosphere, and very small emission features from HO<sub>2</sub> and a heavy (symmetric O<sup>18</sup>O isotope) ozone line. A figure similar to Figure 1 is shown by *Lahoz et al.* [this issue] regarding the emission features relevant to the 183-GHz radiometer, which includes the other primary ozone line as well as the H<sub>2</sub>O line targeted by MLS. The 183-GHz ozone line is 4 times stronger than the 205-GHz line and thus provides better signals for the mesospheric region. It is essentially free of contaminant species, except for the lowermost stratosphere, where H<sub>2</sub>O continuum emission is present. Also, excess radiation (in comparison to model radiances) is measured by MLS in the essentially “line-free” spectral domain of band 3 below about



**Figure 1.** Main spectral features contributing to the Microwave Limb Sounder (MLS) radiances from the 205-GHz radiometer, for typical lower (46 hPa) and upper (4.6 hPa) stratospheric midlatitude conditions. Spectral regions covered for both primary and image sidebands of bands 2 and 3 (for ClO), and band 4 (for ozone) are indicated by vertical dashed lines. Species with significant emission features are indicated. A similar diagram is given by *Lahoz et al.* [this issue], for the H<sub>2</sub>O and 183-GHz O<sub>3</sub> spectral features measured by MLS.

a 30-km tangent height, even in very dry regions of the atmosphere. A contribution from the collision-induced spectrum of molecular nitrogen and oxygen is probably responsible, and this continuum, referred to as “dry air continuum,” has been fitted empirically and included in the calculated radiances for all MLS bands. We discuss in section 5 the potential contribution to ozone mixing ratio errors (systematics) of inaccurate knowledge of the various aforementioned parameters, which can contribute to emission in the ozone band region.

It can be shown [*Waters, 1993*] that the relative contribution to the measured limb emission, for optically thin situations, has a Gaussian distribution along the observation path, with center at the tangent point and width equal to the resolution along the line of sight, perpendicular to the UARS velocity, namely,  $\sim 400$  km. MLS, under normal operations, performs a complete limb scan with radiometric calibrations every 65.536 s, a “MLS major frame” during which one atmospheric profile is retrieved for each species of interest. The limb scan used in normal operations [see *Jarnot et al.*, this issue] consists of discrete steps between about 90- and 0-km tangent heights, with step spacing for the scan varying between  $\sim 1$  km in the lower stratosphere to  $\sim 5$  km in the mesosphere; individual spectra are measured during 1.8-s dwells (“MLS minor frames”) between steps. Calibration of the radiances occurs during each limb scan, when the MLS switching mirror “switches” to views of the internal blackbody target or space (at a temperature of 2.7 K). The UARS orbital motion (7 km/s) during the limb scan smears the profile measurements over  $\sim 400$  km in a direction perpendicular to the MLS line of sight. The FOV vertical extent at the tangent point for the ozone measurements is  $\sim 3$  km, the approximate inherent vertical resolution of the mea-

surements. As discussed below, the MLS Version 3 data are produced on a vertical grid with points spaced each factor of  $10^{1/3}$  (or 2.15) change in atmospheric pressure, giving a vertical resolution of 5.4 km (for a 7-km pressure scale height). Atmospheric pressure at the tangent point of the observation path is simultaneously measured by observations of thermal emission from molecular oxygen, and this provides the vertical coordinate for the profile retrievals.

The measurement latitudinal coverage is from  $34^\circ$  on one side of the equator to  $80^\circ$  on the other. UARS performs a yaw maneuver at  $\sim 36$ -day intervals (a “UARS month”), when MLS high-latitude coverage switches between north and south. Within each UARS month the UARS orbit plane precesses slowly with respect to the Earth-Sun line. The orbit precession causes the measurements to sweep through essentially all local solar times during the course of a UARS month, becoming 20 min earlier each day at a fixed latitude.

### 3. Data Processing

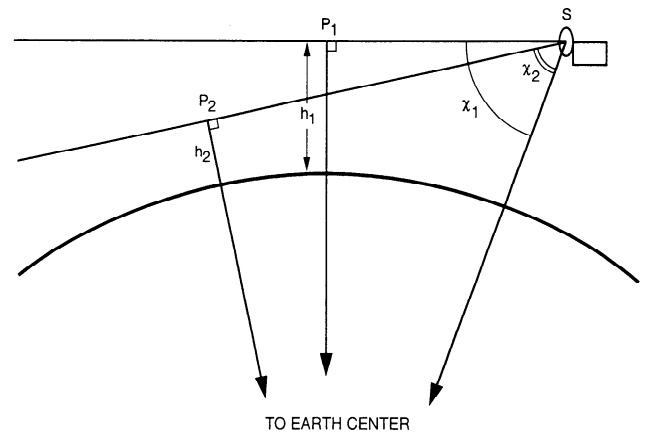
Here, we give a description of the general technique used for all MLS Version 3 retrievals, with some mathematical details given in the Appendix. We also present specifics of the retrievals for Version 3 ozone, which is the focus of most of the remainder of this paper. Retrieval specifics for the other primary MLS products are in companion papers by *Fishbein et al.* [this issue] for tangent pressure and temperature, *Waters et al.* [this issue] for ClO, and *Lahoz et al.* [this issue] for H<sub>2</sub>O.

MLS data processing produces individual files containing measurements made over a 24-hour period, from 0 to 24 hours UT on each day. There are two major steps to the processing. The first converts raw en-

gineering (“Level 0”) data from the instrument telemetry into calibrated radiances and other engineering diagnostics and produces a “Level 1” file. *Jarnot et al.* [this issue] describe the MLS Level 1 processing. The second processing step converts calibrated radiances from daily Level 1 files into geophysical data, producing “Level 2” files (geophysical parameters and estimated uncertainties on a vertical grid chosen by the instrument team). The Level 2 processing step for MLS also produces “Level 3A” files, which are geophysical parameters (one file per parameter) on a vertical grid common to all UARS instruments producing atmospheric profiles. There are two sets of Level 3A files: (1) Level 3AT which has profiles equally spaced in time intervals of 65.536s and (2) Level 3AL which has profiles equally spaced in latitude intervals of 4°. There are typically 1318 or 1319 profiles in each MLS Level 3AT file and about 840 profiles in each MLS Level 3AL file. Additional processing of Level 3AL files (C.A. Reber et al., manuscript in preparation, 1996), produces Level 3B files which contain data commonly gridded in the horizontal for all UARS instruments producing Level 3AL data; these files can be used to generate “synoptic” fields of mean ozone and its wave components, but various investigators are producing their own version of such fields [e.g., *Elson and Froidevaux*, 1993]. Finally, each daily set of MLS Level 3AT and Level 3AL files has an associated Level 3PT and Level 3PL file (named Level 3 parameter files); these files contain additional information, such as diagnostics of the quality of the retrievals for each band, and the overall status of each major frame of MLS data. It is strongly recommended that the latter flag be monitored and used to discard bad data (also detectable by checking the sign and/or magnitude of the estimated uncertainties available in Level 3 files, as described below); although bad data are a rare occurrence on a typical day of MLS data, there are certain days/periods when certain or all MLS measurements are bad or unavailable, yet climatological (a priori) information can still be found in the data files. A brief summary of some of the above issues and other caveats specific to the currently available MLS data files, as well as a complete description of the MLS file contents, is in the Standard Formatted Data Units documentation available from the NASA Goddard Space Flight Center Distributed Access Archive Center (DAAC).

### Retrievals

Figure 2 is a schematic of the UARS MLS measurement geometry. Although not shown in the figure, there are three separate radiometers, each viewing at slightly different elevation angles (due to optical design constraints) for a given scan position reference point, given by the 63-GHz radiometer FOV direction. These angular differences (measured prior to launch; see *Jarnot et al.* [this issue]) are referred to here as  $\delta\chi$  and  $\delta\chi'$  for the 205-GHz and 183-GHz to 63-GHz FOV elevation differences; they correspond to about -290 m and +50 m in tangent altitude difference, respectively. The



**Figure 2.** Schematic of the UARS MLS measurement geometry. The UARS MLS observations are made from point S, where emission from the Earth’s atmosphere (e.g., points P<sub>1</sub> and P<sub>2</sub>) is received, as the MLS antenna scans through the limb.

equation of radiative transfer is used to calculate the radiances originating from various tangent points (e.g., P<sub>1</sub> and P<sub>2</sub> in the figure), as the antenna FOV scans the atmosphere at different elevation angles (e.g.,  $\chi_1$  and  $\chi_2$ ). The calculated limb radiance values are then convolved over the antenna pattern and the channel filter response [see *Jarnot et al.*, this issue; W.G. Read et al., manuscript in preparation, 1996].

The approach used here for retrieving geophysical parameters of interest, such as tangent pressure ( $P_{\text{tan}}$ ), temperature ( $T$ ), and mixing ratios ( $f$ ), from the MLS calibrated radiances (Level 1 data), is based on sequential estimation, as first applied to limb sounding by *Rodgers* [1976]. This technique combines a priori information (such as climatological profiles with an associated error covariance) with measurement information, to produce a solution for the desired parameters, or state vector  $\mathbf{x}$  and associated error covariance matrix  $\mathbf{S}$ . The a priori “state vector” is used to stabilize the solution in regions of poor sensitivity and to provide some continuity. For example, tangent pressure a priori values in regions of poor measurement sensitivity are obtained from the hydrostatic equation relating changes in pressure to changes in height ( $h$ );  $h$  is given by  $(R_S \cos \chi/n) - R_E$ , where  $R_S$  is the Earth center to satellite distance,  $R_E$  is the Earth radius at the sub-tangent point, and  $n$  is the index of refraction at the tangent point. The angular change between  $\chi_1$  and  $\chi_2$  in Figure 2 is largely caused by the antenna scan motion between measurements at different minor frames but also by the spacecraft roll component. These calculations serve as estimates of tangent pressure at heights below 22 hPa (for Version 3 data), where the 63-GHz O<sub>2</sub> line is close to saturation, as well as in the top portion of the atmosphere, where MLS retrievals of  $P_{\text{tan}}$  and  $T$  are not currently reliable [see *Fishbein et al.*, this issue]. Independent parameters such as  $R_S$  and  $R_E$  are therefore part of the state vector, via their effect on the a priori model (or virtual measurement model).

The above methodology can be viewed as a combination of the a priori information and the weighted least squares solution to the linearized equation relating measurements and state vector (see Appendix for a simple derivation).

The update of state vector  $\mathbf{x}$  is obtained using the following sequence of equations [see *Rodgers, 1976*], for each channel radiance  $y_i$  in a given band (or bands), and from top to bottom of the atmosphere:

$$\hat{\mathbf{x}}_i = \hat{\mathbf{x}}_{i-1} + \frac{\hat{\mathbf{S}}_{i-1} \mathbf{K}_i (y_i - y_i^c)}{\mathbf{K}_i^T \hat{\mathbf{S}}_{i-1} \mathbf{K}_i + \epsilon_i^2 + \omega_i^2}, \quad (1)$$

$$\hat{\mathbf{S}}_i = \hat{\mathbf{S}}_{i-1} - \frac{\hat{\mathbf{S}}_{i-1} \mathbf{K}_i \mathbf{K}_i^T \hat{\mathbf{S}}_{i-1}}{\mathbf{K}_i^T \hat{\mathbf{S}}_{i-1} \mathbf{K}_i + \epsilon_i^2 + \omega_i^2} \quad (2)$$

with starting points given by the a priori values  $\hat{\mathbf{x}}_0 = \mathbf{x}_a$  and  $\hat{\mathbf{S}}_0 = \mathbf{S}_a$ ; column vector  $\mathbf{K}_i$  is given by the  $i$ th row of the weighting function matrix  $\mathbf{K} = \partial \mathbf{y}^c / \partial \mathbf{x}$ ,  $\epsilon_i^2$  is the  $i$ th diagonal element of the measurement error covariance matrix (assumed diagonal for the above equations), and  $\omega_i$  is an additional error term discussed below. The calculated radiances  $y_i^c$  and their derivatives  $\mathbf{K}_i$  are obtained by table lookup (for speed of evaluation) from climatological conditions and then interpolated in the vertical to the tangent pressure for  $y_i$ ; atmospheric profiles are tabulated for 10 different months (one per ‘‘UARS month’’), 8 latitude bins (from 70°S to 70°N in 20° increments), 43 tangent pressures (on the UARS L3 grid), and for ascending or descending sides of the orbit (for Doppler shift correction purposes). Radiances are interpolated with respect to (logarithm of) tangent pressure using cubic splines and with respect to other variables via the linearized form (based on tabulated radiances  $\mathbf{y}^c$  and state vector  $\hat{\mathbf{x}}$ ) so that  $y_i^c$  in equation (1) is given by

$$y_i^c = \mathbf{y}_i^c + \mathbf{K}_i (\hat{\mathbf{x}}_{i-1} - \hat{\mathbf{x}}) \quad (3)$$

Given that this tabulated linear model is not as accurate as the complete radiative transfer model, so closure may not be as optimum as desired, we have increased the radiance uncertainties  $\epsilon_i$  by an ‘‘inflator’’ factor equal to 1% of the radiances + 0.75 K for band 1 [see *Fishbein et al.*, this issue] and by 3% of the radiances for bands 4 through 6; the factor was deemed unnecessary for ClO (bands 2 and 3), since the root mean square (rms) noise is large compared to the radiances, in general, in that case. Moreover, the term  $\omega_i^2$  also includes contributions from variables which can affect the state vector components being retrieved for a particular band but which are constrained to values  $\mathbf{x}^c$ , with error covariance  $\mathbf{S}^c$ . These uncertainties, some of which may not be purely random, will contribute an additional factor  $\mathbf{K}_{ci}^T \mathbf{S}_{i-1} \mathbf{K}_{ci}$  as part of  $\omega_i^2$  above. For example, temperature and tangent pressure uncertainties, after their evaluation from band 1 retrievals, have their uncertainties propagated to mixing ratio estimates in this way; also, uncertainties arising from velocities (Doppler shifts) along the FOV direction are treated in this fashion, with no values retrieved, but with the (a priori) uncertainty estimates included in the equations for mixing ratio updates. In terms of the estimated error covariance (whose diagonal elements give the uncertainties in the MLS data files), we note that the retrieval software produces uncertainties which are flagged as negative under conditions of poor measurement sensitivity (see discussion in next subsection for more details).

The order of the retrievals is chosen as band 1 ( $P_{\text{tan}}$  and  $T$ ), since  $P_{\text{tan}}$  is needed first as a vertical coordinate for geophysical parameters and  $T$  is used in the radiance calculations for other bands, band 5 (H<sub>2</sub>O), because of its potential impact on other species, band 6 (ozone), band 4 (ozone), and bands 2 and 3 (ClO). Table 1 provides a list of the state vector components which are either retrieved or constrained, as a function of band

**Table 1.** State Vector Components in MLS Version 3 Retrievals

Radiance Band	Retrieved Components	Constrained Components
B1, 63 GHz	$P_{\text{tan}}, T, y_1^{\text{off}}$	$f^{\text{O}_2}, f^{\text{O}^{18}\text{O}}, v, R_E, R_S, B$
B5, 183 GHz	$f^{\text{H}_2\text{O}}, y_5^{\text{off}}$	$P_{\text{tan}}, T, \delta\chi', v, R_E, R_S$
B6, 183 GHz	$f^{\text{O}_3(183)}, y_6^{\text{off}}$	$P_{\text{tan}}, T, f^{\text{H}_2\text{O}}, \delta\chi', v, R_E, R_S$
B4, 205 GHz	$f^{\text{O}_3(205)}, y_4^{\text{off}}$	$P_{\text{tan}}, T, f^{\text{H}_2\text{O}}, f^{\text{O}^{18}\text{O}}, \delta\chi, v, R_E, R_S$
B2/B3, 205 GHz	$f^{\text{ClO}}, f^{\text{SO}_2}, f^{\text{HNO}_3}, y_{2/3}^{\text{off}}, y_{2/3}^{\text{lin}}$	$P_{\text{tan}}, T, f^{\text{O}_3(205)}, f^{\text{H}_2\text{O}}, f^{\text{H}_2^{18}\text{O}}, f^{\text{O}^{18}\text{O}}, \delta\chi, v, R_E, R_S$

Bold type indicates a vector (like  $T, f, v$ , and  $B$ ), including a quantity which has an updated value for each scan position (like  $P_{\text{tan}}, y^{\text{off}}$ , and  $y^{\text{lin}}$ ).  $R_E$  and  $R_S$  are updated once per major frame (complete scan) for their effect on radiances, but once per minor frame (scan dwell position) in the a priori equation for tangent pressure (see description in text). Mixing ratios ( $f$ ) include the appropriate species as a superscript. Other quantities are defined in the text.

(listed in the above processing order). Among the parameters not mentioned yet are  $\mathbf{B}$ , which represents magnetic field, for its Zeeman splitting effects on the O<sub>2</sub> line in band 1, particularly in the center channels and in the mesosphere [see *Fishbein et al.*, this issue]. Also, we retrieve a set of baseline offsets  $\mathbf{y}^{\text{off}}$  and (for bands 2 and 3) linear coefficients  $\mathbf{y}^{\text{lin}}$ , with one component for each minor frame; the a priori values for these are based on the previous minor frame (but with conservatively large a priori uncertainties). Correlations among these coefficients (and for  $P_{\text{tan}}$  as well) are not rigorously accounted for, since the software overwrites each of these variables after each minor frame; a fuller treatment will be undertaken in future algorithms if necessary, although the effects on mixing ratios are not expected to be very large (based on tests already performed). There are also some parameters which we have not explicitly included in the table but which are implicitly included in the forward model or the a priori model. These include the elevation angle  $\chi$  and satellite roll angle, which enter in the a priori tangent pressure equation (described above), geometric quantities needed to perform transformations between the UARS MLS reference frames and the Earth-centered frame, as well as assumptions for N<sub>2</sub>O, dry air continuum, and a few other trace species in the (tabulated) forward model radiances. We note also that HNO<sub>3</sub> emission contribution in band 4 was included as part of the tabulated forward model radiances (based on climatology), but no HNO<sub>3</sub> retrievals were attempted in Version 3 data.

No attempt is made to include “memory” from one scan profile (or retrieval) to the next [see *Rodgers*, 1976], except through the a priori (tangent pressure evaluation and climatological geophysical parameters). This was done to preserve independence between consecutive profiles (and to minimize propagation of “bad” retrievals) and because it was not obvious from test results that such smoothing (filtering) along the tangent track would give rise to significantly better retrievals. Another important feature of the MLS retrievals used in the production of Version 3 data is the use of an “opacity criterion,” which eliminates radiances corresponding to large optical depths along the line of sight, because of nonlinearity concerns (given the noniterative linear scheme used so far). This is not used for band 1, since a nonlinear calculation of radiances is used for this band. For all other bands, if one ignores the image sideband contribution to the radiance, a particular radiance at frequency  $\nu$  can be written (approximately) as

$$y(\nu) = g_p(\nu) T_{\text{tan}} (1 - e^{-\tau_p(\nu)}) \quad (4)$$

where  $g_p(\nu)$  is the primary sideband gain factor,  $T_{\text{tan}}$  is the tangent point temperature, and  $\tau_p(\nu)$  is the optical depth along the line of sight. This leads to an estimate of the optical depth, given an estimate of  $T_{\text{tan}}$ , from band 1 retrievals, and the measurement  $y(\nu)$ , namely,

$$\tau_p(\nu) = -\ln(1 - y(\nu)/g_p(\nu) T_{\text{tan}}) \quad (5)$$

When this estimated optical depth is greater than unity, the radiance is ignored in the sequential estimate update equations.

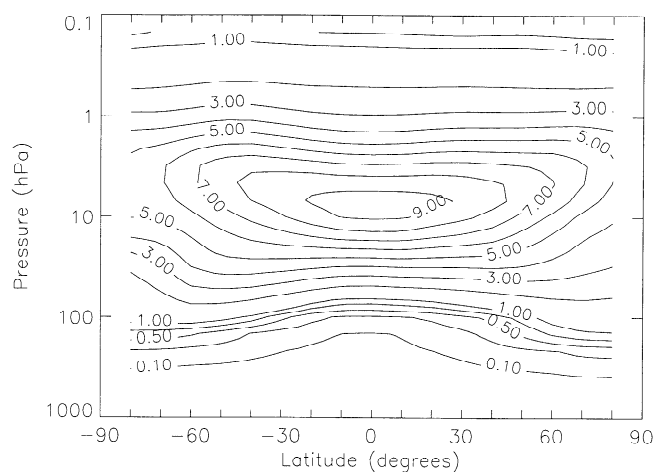
Some of the software features described above are expected to change in future iterative nonlinear retrieval algorithms, where more optimum use can be made of the MLS radiances, with essentially no radiance cutoff criterion, and a reevaluation of the radiance error inflator factors as part of the plans.

### Version 3 Data

The constituent profiles used in Level 2 files for the MLS Version 3 data are represented as piecewise-linear in mixing ratio versus logarithm of atmospheric pressure, with break points at  $1000 \times 10^{-n/3}$  hPa where  $n$  is an integer. For ozone the starting and ending values of  $n$  are 1 and 19, which corresponds to pressures of 464 and  $4.6 \times 10^{-4}$  hPa, respectively; these fixed boundaries were chosen very conservatively. A subset of this vertical range, most useful for scientific analyses, will be recommended below in this paper. The UARS Level 3 pressure grid ( $1000 \times 10^{-n/6}$  hPa values) is twice as fine as the MLS Level 2 grid, and we have simply averaged the adjacent Level 2 grid values to fill in the Level 3 grid on the “odd” UARS surfaces. This leads to a reduction in the variability (e.g., about the zonal mean) for these odd pressure surfaces, compared to the even surfaces, since the averaging process reduces random noise.

The error factor added to the radiances (see the subsection on retrievals above) to account for some of the forward modeling uncertainties was set at 3% of the radiances in both ozone bands. The opacity criterion used to discard radiances because of nonlinearity effects was set to unity. Finally, it was found from simulations that better retrievals were obtained if radiances arising from tangent pressures larger than 100 hPa were not included, at least for the noniterative retrievals used to produce Version 3 data. A more optimum use of all channels will be sought in future software upgrades.

An example of the a priori values used for ozone is given in Figure 3, for the month of September. The ozone climatology file was provided by members of the UARS community, based on values given by *Keating et al.* [1989a,b], with extrapolations for the poorly represented lower stratosphere (at pressures over 20 hPa). Model values from the Lawrence Livermore National Laboratory two-dimensional model were used to fill in the tropospheric “climatology;” remaining missing data in the mesosphere and above were filled in with standard middle-latitude values from the Caltech/Jet Propulsion Laboratory one-dimensional photochemical model. A priori uncertainties are generally chosen conservatively (i.e., large values are used) in order to minimize possible biases. For ozone a 3 parts per million by volume (ppmv) a priori uncertainty is used in the stratosphere down to 50 hPa, with a 2 ppmv uncertainty at 100 hPa, and significantly tighter constraints in the troposphere, where no attempt is currently being made to retrieve ozone (climatological fields are found there in the MLS data files). A priori uncertainties decrease



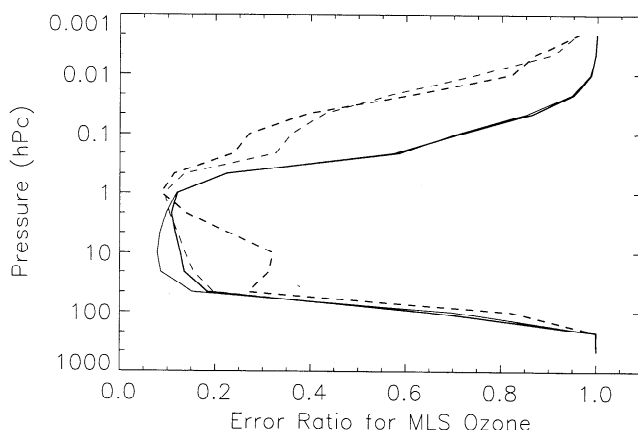
**Figure 3.** September zonal mean cross section for climatological ozone (ppmv) used as a priori information (see text) in the retrieval algorithms.

smoothly with decreasing pressure in the mesosphere, until about 0.2 hPa, above which an uncertainty of 1 ppmv is assumed. Based on sensitivity tests of the influence of a priori values, we find that the 205-GHz ozone retrievals are affected in a nonnegligible way by the a priori for pressures near 100 hPa and above about 0.46 hPa; for the 183-GHz retrievals, these boundaries are near 46 hPa and above about 0.046 hPa. The use of a “global” a priori uncertainty is clearly an oversimplification of the variability of the real atmosphere. The possibility of larger—than—appropriate estimated uncertainties in the retrieved profiles exists as a result of this approach, for regions like the lowermost stratosphere where poorer measurement sensitivity exists (see section 5); however, this is a safer approach than the use of a priori uncertainties which are too small, since this can lead to undesirable biases with unrealistically small estimated uncertainties.

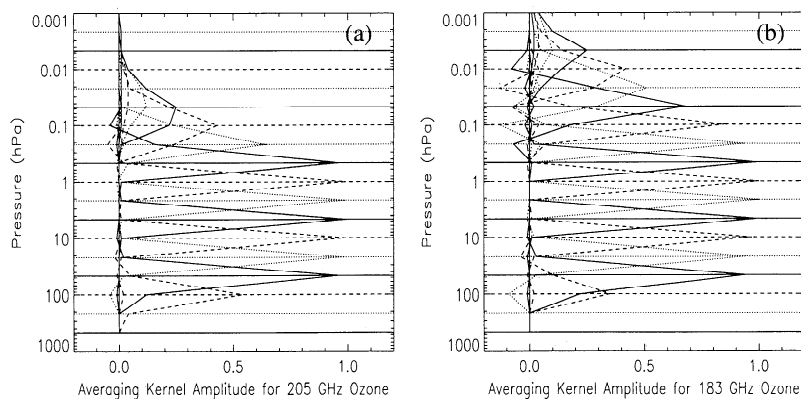
As mentioned in the previous subsection, a diagnostic of the relative sensitivity of measurements and a priori can be obtained by considering the ratio of estimated uncertainty (in the retrieval product) to the a priori uncertainty. Typical (average) values of this “error ratio” are shown in Figure 4 for both ozone retrievals at two selected latitudes, on September 17, 1992. This function is characterized by values near unity where no measurement information exists, values close to zero (about 0.1 to 0.3 here) where significant measurement information exists, and a steep gradient in the transition regions where an increasing contribution comes from the a priori. Figure 4 shows that below  $\sim 1$  hPa, ozone from the 205-GHz radiometer provides a slightly more sensitive measurement than the 183-GHz data (for Version 3 results). Above 1 hPa the 183-GHz ozone measurements become increasingly more sensitive in comparison to the 205-GHz retrievals; thus the 183-GHz data are recommended for studies of mesospheric ozone, even if the expected accuracy is less than for the 205-GHz ozone (see section 5).

The “error ratio” is used to qualify retrieved values in the MLS data files. When the error ratio is greater than 0.5 (a fairly conservative value, within the steeply increasing region of Figure 4), which means that the a priori contributes more than 25% to the result and the measurement-related uncertainty is more than  $1/\sqrt{3}$  (or 0.58) times the a priori uncertainty, the estimated uncertainties are flagged with a negative sign. This alerts the user that poorer measurement sensitivity is expected, and the use of data values in these regions is cautioned against, since essentially, no MLS measurement information exists beyond the flagged boundaries. The Version 3 data show variations in error ratio versus latitude, particularly for the 183-GHz ozone results, because more channels are being discarded from the retrieval process near the equator in the midstratosphere. Future algorithms will avoid this by iterating over the retrieval process until convergence is reached, thereby allowing all channels to be used to their fullest potential. Such issues are less critical in Version 3 205-GHz results, since essentially all channels are always being used in the current algorithms; however, some improvements may be obtained via more accurate retrievals of other parameters (such as tangent pressure, temperature, and H<sub>2</sub>O) which can have some impact on the ozone values (see section 5).

Averaging kernels are another, more formal expression of measurement sensitivity used in the description of error characterization [see Rodgers, 1990; Marks and Rodgers, 1993]. The rows of the averaging kernel matrix represent height-dependent weighting factors by which the true atmospheric profile is multiplied to give the retrieved profile. These functions are given in Figure 5 for MLS ozone retrievals representative of Version 3 data, in both frequency bands. The kernels provide a measure of profile sensitivity to changes in the true profiles and are equal to unity if no a priori influence exists; their vertical widths give a measure of vertical resolution (smoothing of the true profiles). These fig-



**Figure 4.** Error ratio (estimated over a priori) for MLS ozone retrievals at 70S latitude (thin lines) and at the equator (thick lines); solid lines are for 205-GHz results, dashed lines are for 183-GHz results (both for September 17, 1992).



**Figure 5.** Averaging kernels (see text) of MLS Version 3 ozone retrievals for (a) 205-GHz data and (b) 183-GHz data.

ures confirm the information provided above, regarding the relative sensitivity of 205- and 183-GHz retrievals in the current MLS algorithms. Some degradation in measurement sensitivity can be seen in the lower mesosphere and at 100 hPa for the 205-GHz ozone data. The sensitivity is slightly worse for the 183-GHz results at 100 hPa and also at altitudes somewhat above this (e.g., in equatorial regions, see Figure 4; note that the kernels in Figure 5 are for midlatitudes). The larger values of averaging kernels for the 183-GHz data in the mesosphere imply greater sensitivity in that region than for the 205-GHz data (see also Figure 4). We note that most of the smoothing arising from the MLS measurements is caused by the use of the retrieval grid (not by the instrument FOV or radiative transfer smearing). Also, the averaging kernels shown here were calculated using a representation of the true atmospheric profiles identical to the relatively coarse MLS retrieval grid. Use of a finer resolution true profile will yield somewhat different averaging kernels. This issue is taken up again in section 5 on estimated uncertainties.

#### 4. Radiances and Closure

In this section we examine the MLS ozone radiances, both from simulations performed in an identical fashion to those producing Version 3 data and from the actual data. The issue of closure is discussed by analyzing radiance residuals (observed or simulated radiances minus radiances calculated from the retrieved profiles), as well as diagnostics related to the goodness of fit for these radiances. Furthermore, profile residuals can also provide information on retrieval quality, in the case of simulations. For the production retrievals we discuss known artifacts and caveats (with more information in section 6, based on comparisons with other data sets).

##### Simulation results

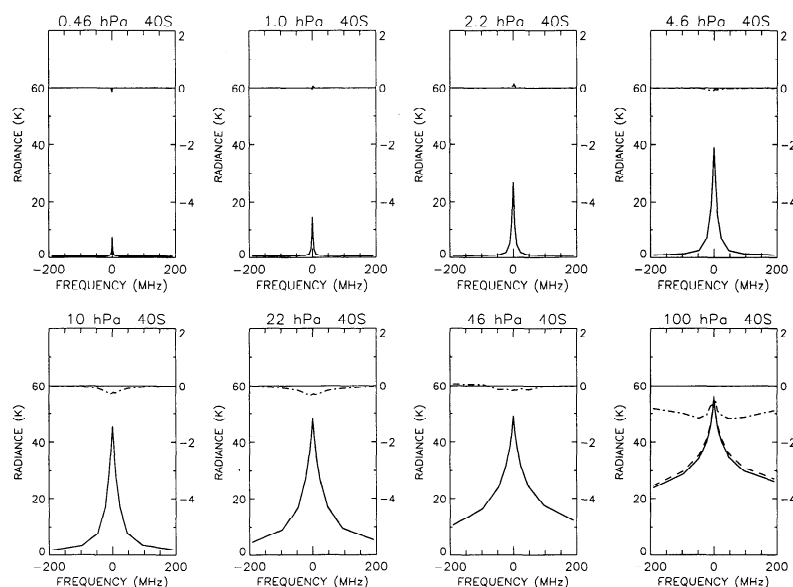
This subsection describes results of simulation studies, in order to understand “numerical errors” arising from the software used to create the Version 3 data files. We do not expect this software to be completely optimum, since it is based on assumptions of linearity

and does not fully utilize the complete set of measurements, which leads to some limitations (particularly in the lowermost stratosphere). More computer-intensive retrievals are needed for a fully iterative (nonlinear) retrieval scheme, now in preparation.

**Radiances and residuals.** The radiance residuals have been calculated based on a set of profiles obtained by smoothing actual MLS-retrieved values for September 17 1992, a day with “ozone hole” conditions in the southern polar regions. The simulation uses the operational MLS scan sequence.

Results from a full day of radiance residuals have been examined in 10 degree latitude bins as a function of pressure, and a typical subset, for 40°S (latitudes 45°S to 35°S) is shown in Figure 6. The results are similar in other latitude bins. We see that closure exists at a level of 1% (of radiances) or better (i.e., less than  $\sim 0.2$  K), except at the lowermost pressure shown (100 hPa), where the calculated radiances are systematically higher by about 1 K than the “observed” radiances (which are of the order of 20 to 60 K). While this is not a large percentage difference in radiances, retrievals of ozone in the lowermost stratosphere depend more heavily on radiances (or radiance differences) in the outside (wing) channels, and spectral differences introduced between model and observed radiances have the potential to significantly impact ozone values near 100 hPa. As mentioned in section 3, the measurement information, relative to the a priori, is decreasing in the lowermost stratosphere, and this has an impact on the poorer radiance fits obtained there. Better closure has been obtained with test retrievals using a fully iterative method and improved algorithms. The quality of simulated ozone profiles is discussed further below. Figure 7 is similar to Figure 6 but for the 183-GHz ozone results. Although reasonably good radiance fits are also evident in these simulations, they are somewhat worse than those for 205-GHz. The fit at 100 hPa is not an accurate reflection of the actual sensitivity, because we know that the current retrieval scheme has poor sensitivity at that level for the 183-GHz data; the strong influence of climatology thus constrains the agreement between simulated and retrieved ozone fields (and the corresponding radiances).



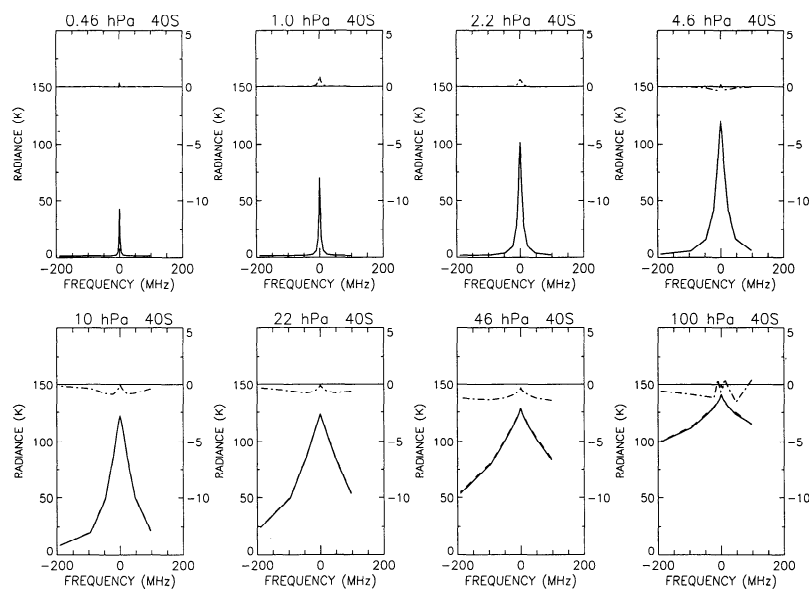


**Figure 6.** Simulated radiances and residuals for MLS 205-GHz ozone. The simulations use smoothed MLS retrievals from September 17, 1992, as input (“truth”). Average results for a 10°-wide latitude bin centered at 40°S are shown. Signals are interpolated onto the MLS retrieval pressure grid and shown for tangent pressures from 0.46 hPa (top left-hand panel) down to 100 hPa (bottom right-hand panel). “Observed” radiances (K) from the synthetic profiles are drawn as solid lines versus frequency from the center channel (in MegaHertz); dashed lines give the “calculated” radiances, based on retrievals from the “observed” radiances, although the two radiance curves are often indistinguishable on the scale shown. Radiance residuals (“observed” minus “calculated”) are displayed about the horizontal “zero line,” based on the right-axis scale (expanded relative to radiance scale by a factor of 10).

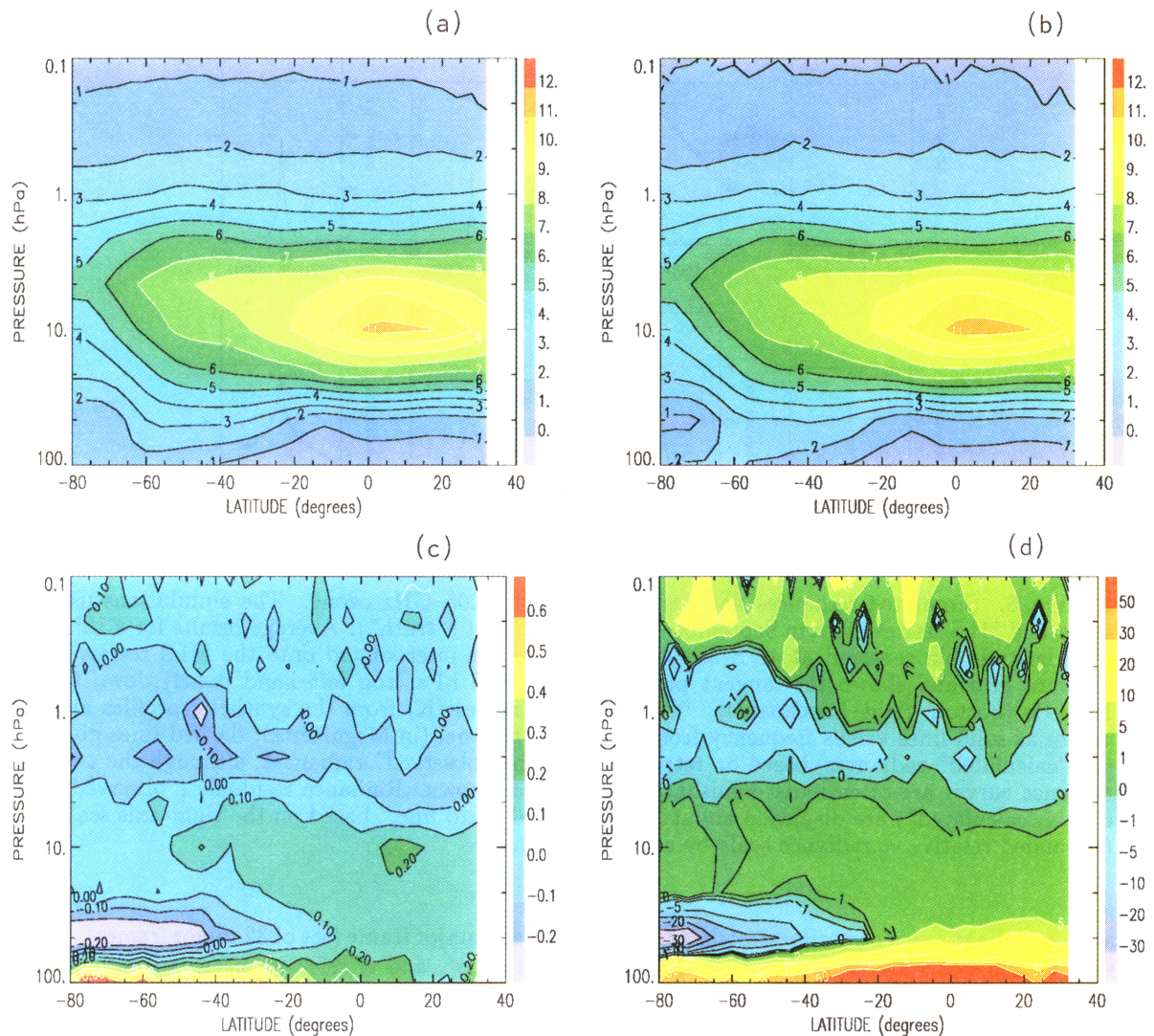
One can define diagnostics of goodness of fit by using the chi-square ( $\chi^2$ ) concepts from statistical analysis [e.g., Bevington, 1969]. We have calculated values of

$$\chi_{ma}^2 = \frac{1}{N} \sum \frac{(y_i - y_i^c)^2}{\epsilon_i^2} \quad (6)$$

for each major frame (set of 32 minor frames). The variables  $y_i$ ,  $y_i^c$ , and  $\epsilon_i$  refer to measured radiance, calculated radiance (linear model used in the retrievals), and random (rms) radiance uncertainty.  $N$  is given by the number of degrees of freedom, namely, the total number of observations (radiances) minus the number of param-



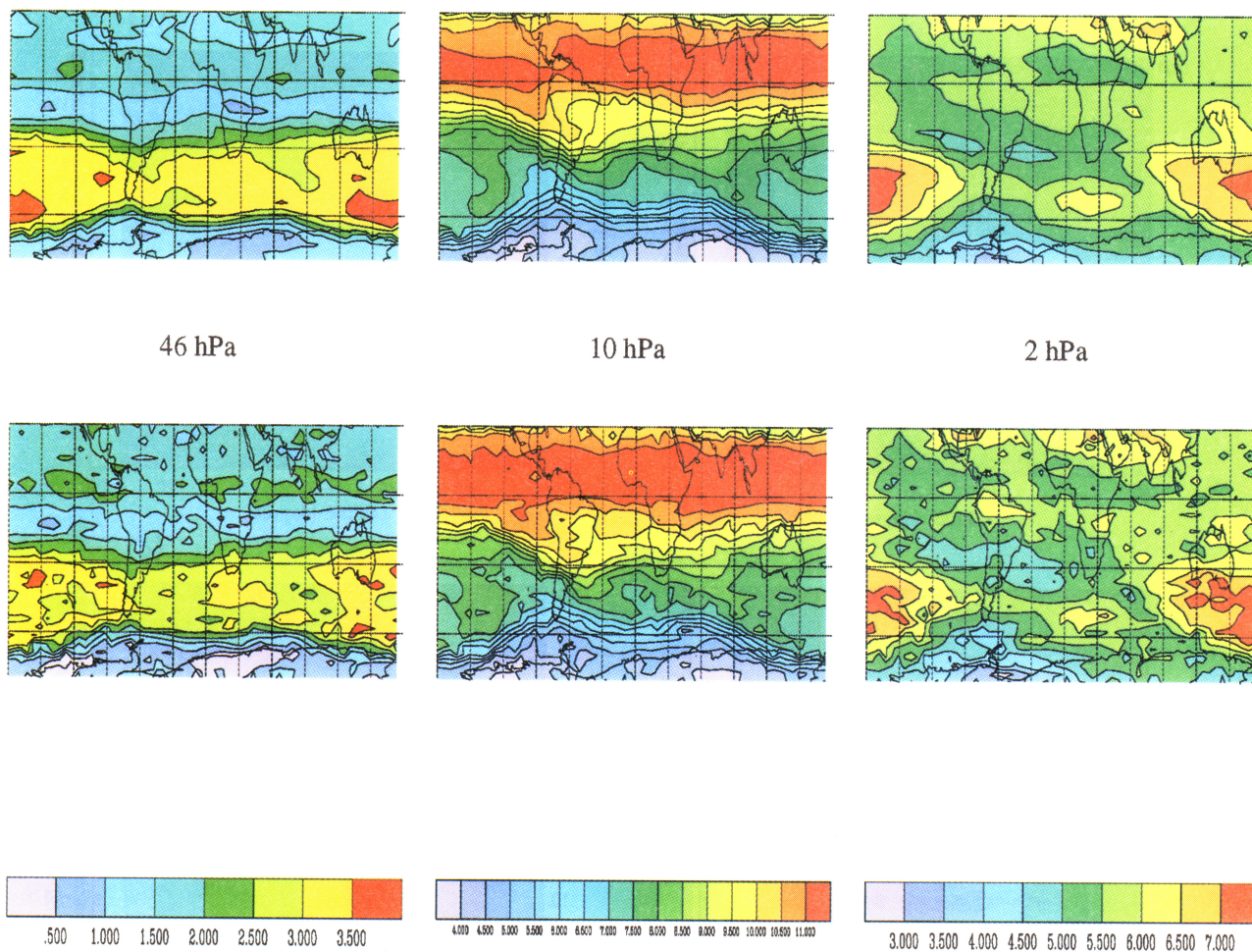
**Figure 7.** Same as Figure 6, but for MLS 183-GHz ozone (with different radiance scale but still a factor of 10 expanded scale on the right axis for residuals).



**Plate 1.** Contour plots (versus pressure and latitude) of zonal mean ozone simulations for MLS retrievals from the 205-GHz band. (a) simulated “true” ozone (ppmv), (b) retrieved ozone (ppmv) based on a set of model radiances (with noise), generated from the “true” profiles, (c) mean differences (ppmv), retrieved minus “true” profiles, (d) mean percent differences; large percentage differences exist at 100 hPa partly because mixing ratios can be very small.

eters being retrieved. The above diagnostic is referred to as a reduced chi square; in the algorithms used to produce Version 3 data files, index  $i$  runs over all radiances from the top of the atmosphere to 46-hPa tangent pressure, to avoid too much emphasis on the less well-characterized regions in the lowermost stratosphere (we may carry these diagnostics down to 100 hPa in future production algorithms). Too large (or too small) a value of  $\chi_{ma}^2$  indicates a poor fit and/or a problem of some kind in the retrievals or measurements. Based on statistics from idealized Gaussian distributions, we have determined that  $\chi_{ma}^2$  values above about 2, given the number of degrees of freedom available for each MLS major frame, are cause for concern and truly indicate poor fits. A similar quantity is also calculated for each minor frame, with index  $i$  running over all 15 channels (14 for ozone at 183-GHz since one of the wing channels is not reliable and is not used); we denote

this diagnostic by  $\chi_{mi}^2$ . The  $\chi_{mi}^2$  values are marginally significant, since the number of measurements is fairly small, but we view these diagnostics as qualitatively useful nevertheless, especially in a relative sense (from minor frame to minor frame, or for different software runs). Zonal mean values of  $\chi_{ma}^2$  and  $\chi_{mi}^2$  are given in Figure 8 for the simulation run mentioned above; radiances with noise similar to the actual instrument noise were used, for a meaningful calculation of  $\chi^2$  diagnostics. From the  $\chi_{mi}^2$  values we observe that the quality of radiance fits degrades in the lowermost stratosphere, particularly in the south polar vortex (south of 60°S). Also, the 183-GHz ozone radiance fits are of relatively poorer quality than the 205-GHz fits, especially close to 46 hPa, consistent with the radiance fit quality observed in previous figures. The values of  $\chi_{ma}^2$  in the bottom panels of Figure 8 follow the average latitudinal trends of the  $\chi_{mi}^2$  values, as expected. Values of  $\chi_{ma}^2$  between



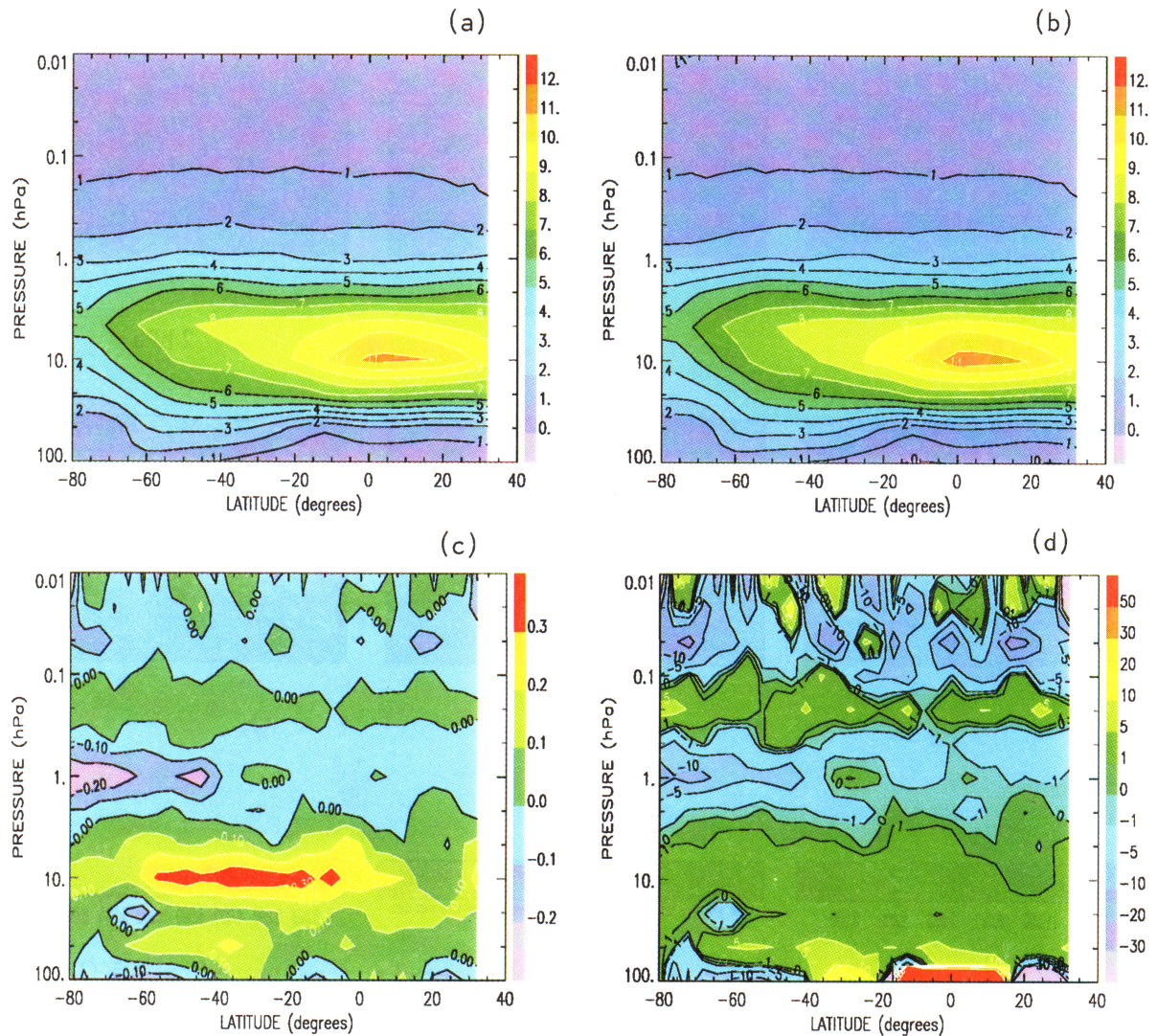
**Plate 2.** Maps of ozone (ppmv) for “true ozone” (top row) and retrieved ozone from 205-GHz simulations (bottom row), with realistic radiance noise, at 46, 10, and 2 hPa (as indicated).

1 and 2 are typical for 205-GHz ozone results (average value is near 1.2). Values between 1.5 and 2 are more typical for 183-GHz ozone, with extrema slightly above 3 (although some larger values exist near the latitude extremes). These results give some lower bounds for the fit quality we may expect in terms of closure based on real data (discussed further below). We will improve upon the simulation results in future software algorithms.

**Ozone abundances.** Retrieved zonal mean fields of 205-GHz ozone are compared to the input (“true”) fields in Plate 1. Zonal mean differences are shown to be  $\sim 0.1$  ppmv or less throughout most of the stratosphere. There is a tendency to underestimate the mixing ratios near 46 hPa and overestimate them at 100 hPa, especially at high latitudes (where the mean biases are of the order of  $-0.4$  and  $0.6$  ppmv, respectively). This translates into  $\sim 20\%$  negative bias in the polar vortex at 46 hPa; at 100 hPa, percentage differences are large, but not so meaningful, because the mixing ratios can become very small, especially in the tropics, but we have to keep these retrieval biases in mind, particularly at high latitudes. We expect to better understand and remove much of these effects in a future data process-

ing, since some of this is undoubtedly related to non-linear effects (in ozone and/or other parameters which contribute to emission in the ozone band). However, between 0.46 and 22 hPa, the true and retrieved ozone fields differ by less than 2%. The retrieved values near 0.2 hPa become clearly influenced by the a priori values, based on our analyses (see also section 5 below).

Another method of examining the retrieval quality is in terms of the reproducibility of “horizontal” atmospheric features, namely, via mapping (simple horizontal gridding in this case) of the Level 3AT ozone fields. We show “true” versus retrieved ozone maps in Plate 2, for pressures of 46, 10, and 2 hPa; the retrievals are from radiances with simulated noise. The differences at these pressure levels arise from noise as well as underlying systematics (exemplified in the zonal mean differences of Plate 1). General features and mixing ratio gradients (e.g., at the edge of the Antarctic vortex and in the subtropics) are very well reproduced. However, there are some features (especially near the boundaries of color contour values) which can lose some of their continuity or appear slightly different after small biases and noise effects are “applied” via the retrieval process. If data users are aware of the noise level and any artifacts or



**Plate 3.** Same as Plate 1 but for zonal mean comparison of simulated ozone from the 183-GHz band with “true” ozone (note that pressure scale extends to 0.01 hPa).

potential biases (as discussed throughout this paper), overinterpretation of maps or MLS results in general should not be a problem.

Plate 3 is similar to the zonal mean cross section comparisons of Plate 1, but for the 183-GHz results. Overall, somewhat better closure is obtained (in comparison with the 205-GHz ozone retrievals) in the mesosphere, with some evidence for degradation (in percentage terms) at pressures less than 0.1 hPa. Less of a bias (than in Plate 1) exists near 100 hPa, but we mentioned earlier that some of this may be an artificial result because of too tight a constraint toward the a priori (as not enough channels are used). Note that a similar percentage fit to ozone will result in a poorer (larger) value of the  $\chi^2$  diagnostic defined above, because the rms radiance noise is comparable for both ozone bands, but the signal is roughly twice as strong for the 183-GHz line (leading to a factor of 4 difference in  $\chi^2$  for a given percentage ozone fit). This is a reflection of the fact that the 183-GHz ozone data are inherently more precise, in a relative sense, and therefore “harder to fit”

to within the noise. Based on these results (and other studies not shown here), the upper limit for 183-GHz ozone data usefulness is near 0.05 hPa (see section 5), and the recommended lower limit is 46 hPa.

### Version 3 Results

This subsection deals with Version 3 results and compares radiance residuals and other diagnostics to simulation values. Known artifacts are also mentioned.

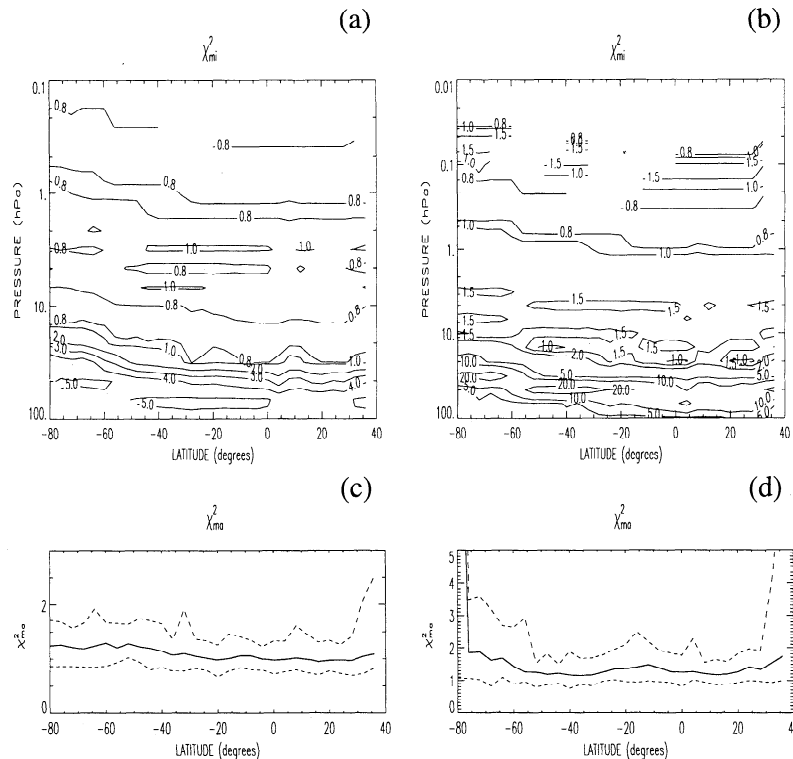
**Radiances and residuals.** Figure 9 shows radiances and residuals for September 17, 1992, at 40°S (similar to the simulations of Figure 6). Residuals are only slightly worse than those from the simulations, except at 46 hPa. Given that the averaging of radiances leads to negligible (0.02 to 0.1 K) noise in the mean radiances, the residual differences are an indication of residual (systematic) errors. There is also some latitudinal variability in the residuals (more pronounced than in the simulation case). For example, we show in Figure 10 some of the poorer fits in the lowermost stratosphere, for 10°S and 70°S. The systematic trends in the

residuals at 46 and 100 hPa are believed to be caused by inaccuracies in the emission features from HNO<sub>3</sub> (on the positive frequency end) and N<sub>2</sub>O (on the negative frequency end); indeed, radiance fits have been found to be significantly improved when HNO<sub>3</sub> is retrieved (but this was not done in the Version 3 data). Also, imperfect knowledge of N<sub>2</sub>O (and H<sub>2</sub>O) in the lowermost stratosphere and upper troposphere will probably have some small effect on the radiance residuals. In summary, poorer radiance residuals are observed in the lowermost stratosphere, but improvements can be expected in future data versions.

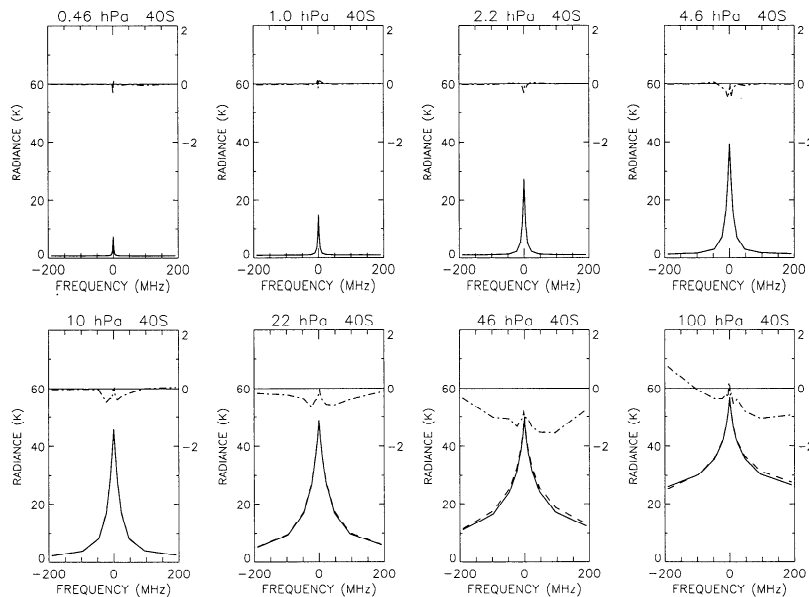
Figure 11 is similar to Figure 9, but for 183-GHz ozone results for September 17, 1992, at 40°S. The radiance residuals are of poorer quality than the 205-GHz ozone results for all pressure levels. At 100 hPa in particular, these plots confirm that little sensitivity exists and that we are attempting to fit climatological radiances (since the retrieval does not perturb the a priori state significantly) to observations. Also, the residual patterns are different than those of Figure 9. Part of the systematic effects in the upper stratosphere (which appear to have a different origin than the asymmetric residuals in the lower stratosphere) may have to do with a slight lack of closure between the forward model runs used in the retrieval and calculated radiance programs. It would seem (from preliminary tests with a fully it-

erative retrieval scheme) that a significant part of the systematic effects observed here are not caused by the linear retrieval scheme's limitations. Therefore instrumental or forward model errors probably have to be invoked. Figure 12 is also similar to the 205-GHz figure above (Figure 10), for radiances and residuals at 10°S and 70°S in the lower stratosphere, at tangent pressures of 22 and 46 hPa. Residuals are maximized at high latitudes at 46 hPa. It would appear from these radiances that the retrieved values from 183-GHz ozone data are too large near 70°S latitude, thus leading to too strong a calculated signal, compared to the measured radiances. The future use of all channels in band 6 should help alleviate some of these lower stratospheric issues for 183-GHz ozone data. Also, we will see in section 8 that updated retrievals using newer spectroscopic data for O<sub>2</sub> (MLS band 1) reduce the radiance residuals.

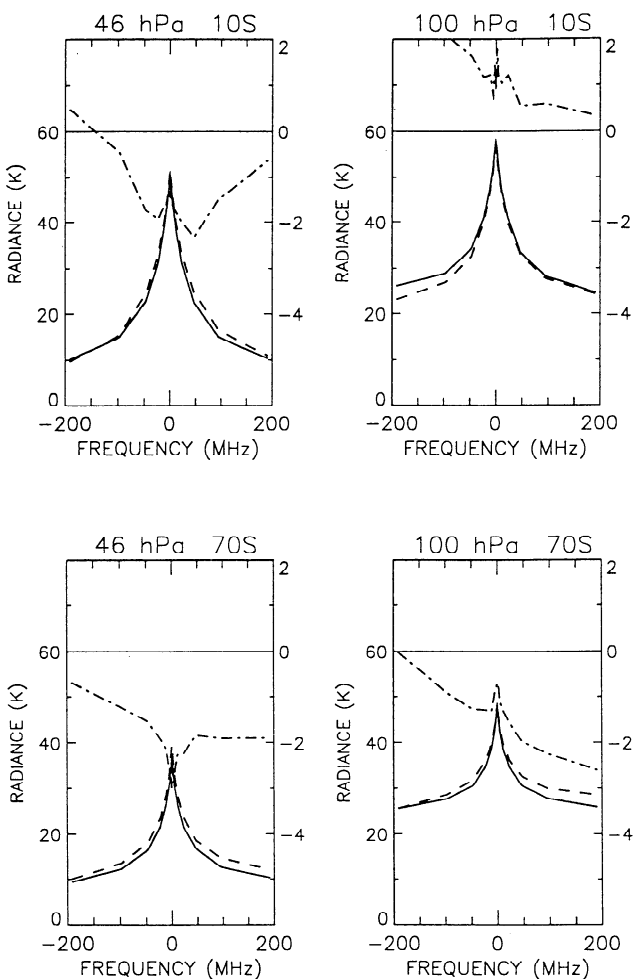
Figure 13 has the same format as Figure 8 (simulations) and provides a measure of the mean goodness of fit ( $\chi_{mi}^2$  and  $\chi_{ma}^2$ ) for both ozone bands, on September 17, 1992. The 205-GHz band results are only slightly worse than the simulation results, and while there is some room for improvement, the fits are judged to be of overall high quality (with increasing problems in the lowermost stratosphere). For the 183-GHz ozone band, however, the goodness of fit is clearly degraded with respect to both the 205-GHz data and the simulation



**Figure 8.** Contour plots of  $\chi^2$  statistics (goodness of fit) for radiances in the 205-GHz ozone band (left-hand panels), and the 183-GHz ozone band (right-hand panels), for the simulated data discussed in relation to Figures 6 and 7. (a and b) Zonal mean values of  $\chi_{mi}^2$  (see text) versus tangent pressure. (c and d) Zonal mean values of  $\chi_{ma}^2$  (see text), solid line, with minimum and maximum values given by dashed lines.



**Figure 9.** Radiances and residuals for MLS 205-GHz ozone in the 40°S latitude bin on September 17, 1992 (actual data, not a simulation). Format used here is identical to that in Figure 6.



**Figure 10.** Radiances and residuals for MLS 205-GHz ozone in the lowermost stratosphere (46 hPa on the left, 100 hPa on the right), at 10°S (top two panels) and 70°S (bottom two panels), on September 17, 1992. Format used here is identical to that used in Figures 9 and 6.

results for 183-GHz ozone, as implied by the radiance residuals discussed above.

Plate 4 shows the time evolution of the zonal mean goodness of fit diagnostic  $\chi_{ma}^2$  as a function of latitude, over the first two years of MLS data acquisition. While we have not identified the cause for poorer residuals at all times and places, this should help caution the data user to be somewhat more careful when the fits are poorer. We believe that the poorer radiance fits in the tropics and midlatitudes in November 1992 and a few other times in the following year are related to the generation of excess instrumental noise induced by the switching mirror movement at low UARS power supply voltages (a problem now circumvented); this also affects the ClO radiance fits [see *Waters et al.*, this issue], and to a lesser extent, the 183-GHz radiometer data. Also, the 205-GHz ozone residuals are poorer than average near 60°S during June/July (early winter), possibly in relation to actual atmospheric variability (and horizontal gradients effects). Somewhat poor fits are also obtained in the tropics during the first 7 months of the UARS mission; this appears to correlate with the poorer comparisons versus tropical ozonesondes in the time period closest to launch (see section 6). The exact cause of these effects remains to be explained (see section 6 for a little more discussion with regard to correlative data). The poorer quality (in an absolute sense) of radiance fits for the 183-GHz ozone data is again evident in Plate 4 (bottom panels). The pattern of tropical and subtropical high ( $\chi_{ma}^2$ ) values appears to follow the pattern of zonal mean ozone obtained in the 205-GHz data [see *Froidevaux et al.*, 1994]. We interpret this to mean that the 183-GHz ozone retrievals cannot (for lack of sensitivity in the current scheme) track the ozone 205-GHz pattern, and this leads to poorer radiance closure. The apparently better closure during the first month of operation is a result of the smaller amount of measure-

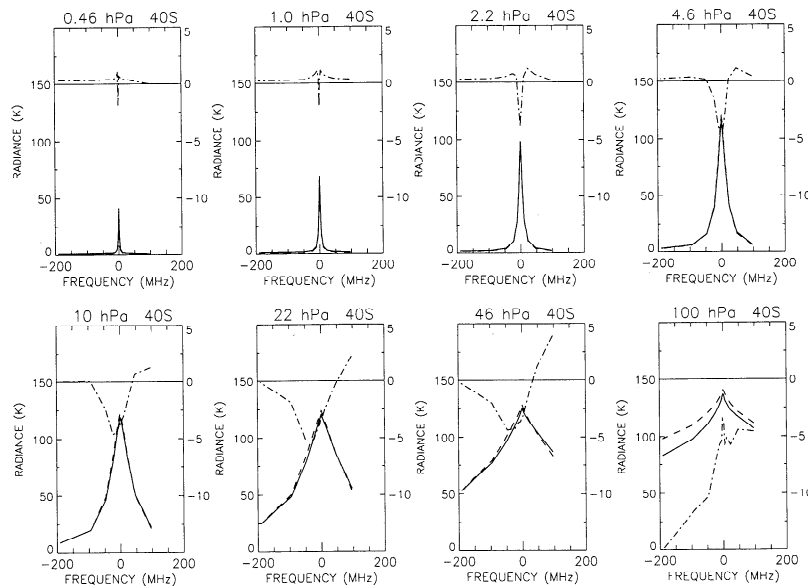


Figure 11. Same as Figure 9 but for MLS 183-GHz ozone.

ments in the lower stratosphere during that initial time period; poorer fits in that region lead to an increase in  $\chi^2_{ma}$  when denser sampling (with more weight in the lower stratosphere) is used.

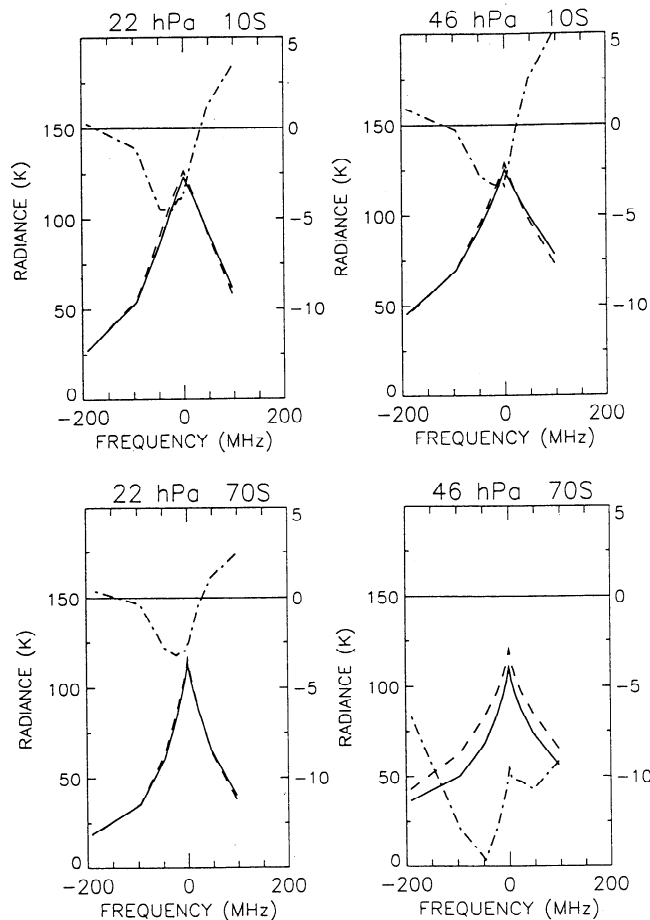
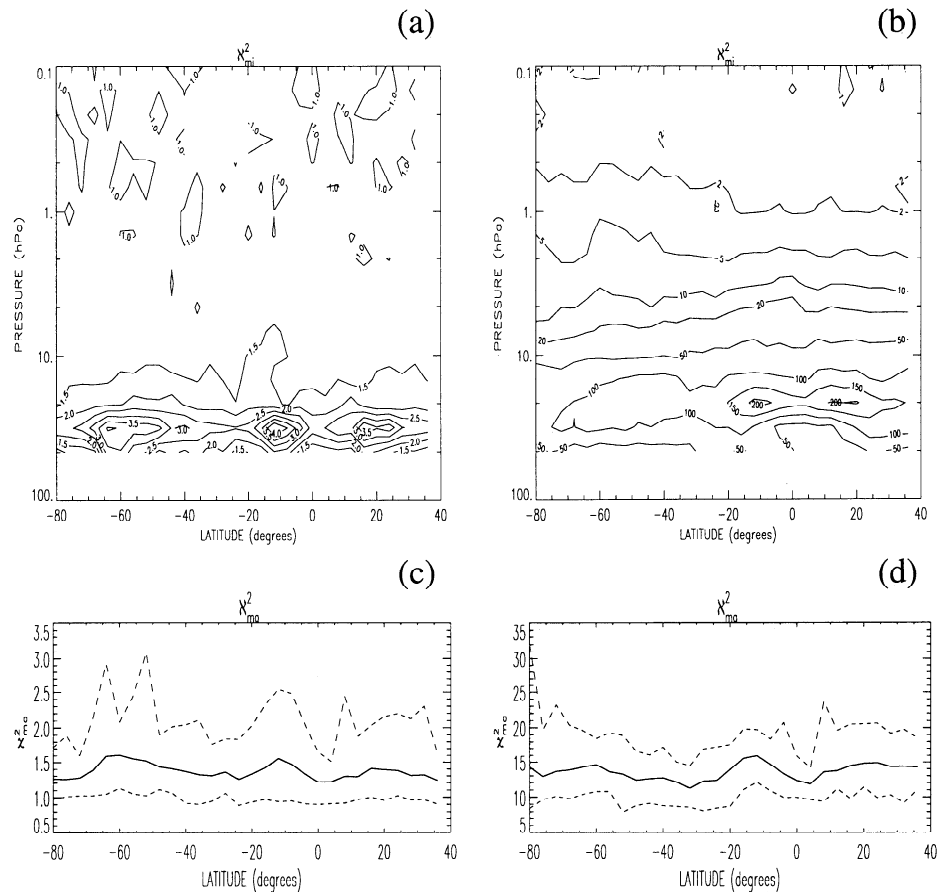


Figure 12. Same as Figure 10 but for MLS 183-GHz ozone and for 46 and 22 hPa rather than 100 and 46 hPa.

**Ozone abundances.** Despite some remaining issues mentioned above, the overall behavior of ozone radiances for the 205-GHz data points to good quality in the results. To confirm this reasonableness issue, Figure 14 shows zonal mean MLS ozone data (from the 205-GHz band) versus climatology, for January and July at various latitudes. The climatological changes in ozone with latitude and season are quite well reproduced by the MLS data. The main difference occurs at 60°S, where the ozone minimum observed near 10 hPa during July is only a weak feature in the climatology; this may have to do with the different vertical resolution of data sets being compared here and warrants further investigation (the MLS minimum is not an isolated incident and exists in 1992 and 1993, for example). More detailed comparisons with correlative data sets are discussed in section 6, in order to assess (or confirm) the quality of MLS retrievals.

**Known artifacts in Version 3 data.** Here, we give a summary of known artifacts associated with the MLS Version 3 ozone data (as also briefly mentioned by Froidevaux *et al.* [1994]); further work is required to better understand these problems and deal with them.

Ozone at 100 hPa has been consistently difficult to retrieve very accurately, probably because of a combination of reduced spectral signature arising from this altitude region and the difficulty associated with modeling (or retrieving) the underlying baseline. The poorer retrievals at 100 hPa are particularly evident during the summer in the tropics, where negative zonal means (of the order of a few tenths of a part per million by volume) persist. Some of these biases could be related to nonlinearity issues, or maybe to the difficulty associated with fitting an inverted profile with a set of coefficients spaced roughly every 5 km. Also, we have observed “bulges” in the mixing ratio at 100 hPa, where the mixing ratios can become unreasonably large (as much as 1 to 2 ppmv), even in a zonal mean, at high south-



**Figure 13.** Contour plots of  $\chi^2$  goodness of fit (radiance) diagnostic for 205-GHz ozone (left-hand panels) and 183-GHz ozone (right-hand panels). Format is identical to that of Figure 8, but actual data for September 17, 1992 are used here rather than simulated data.

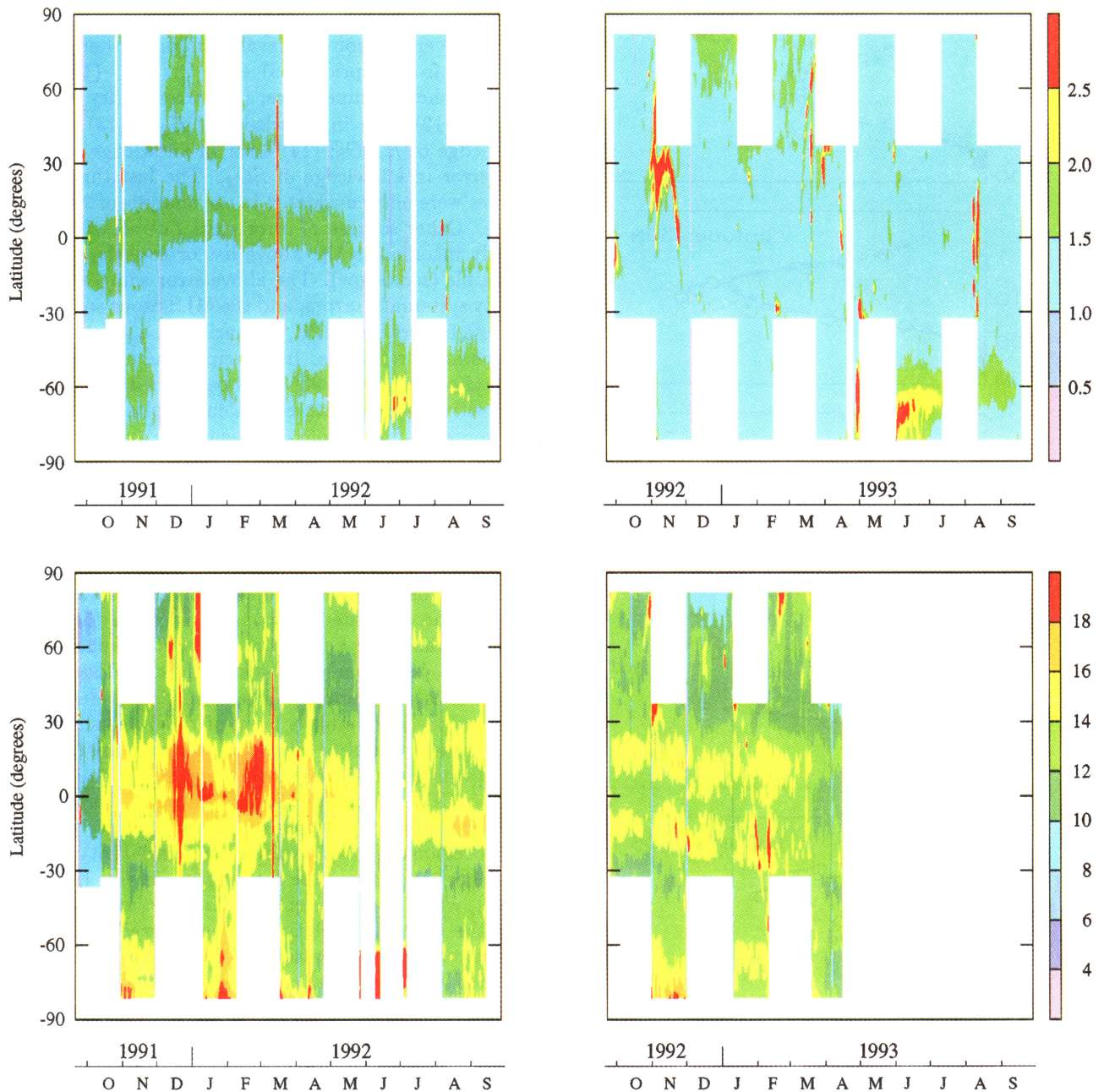
ern latitudes in particular. This effect is exemplified in Plate 5, where we give a map of the difference between the mixing ratio (from the 205-GHz ozone) at 46 hPa and 100 hPa; this difference should typically be positive, but the plots illustrate that there are significant regions where the MLS data yield negative values for this quantity (tropics and high latitudes in particular). These occurrences and the possible underestimate which can follow at the 46-hPa level may be related to the regions of poor radiance closure (see Plate 4 above). Correlative data comparisons confirm that such “bulges” at 100 hPa are not reproduced by ozonesonde data, for example, in the southern polar vortex (see section 6).

The 100-hPa level also exhibits a UARS yaw-cycle dependence (see evidence in Froidevaux *et al.* [1994]); specifically, the mixing ratios (and column values) tend to be larger in the middle of the UARS month. This oscillation (which can be of the order of a few tenths of a part per million by volume) may be related to similar effects observed in temperature [Fishbein *et al.*, this issue] and in lower stratospheric H<sub>2</sub>O [Lahoz *et al.*, this issue]. Efforts to reduce or remove this artifact are continuing, with investigations into better schemes for removing effects apparently caused by baseline offset variations but with no complete explanation or resolution yet. Also,

as yet unexplained occasional “jumps” in mixing ratios exist across yaw days, particularly at the 100-hPa level. We are investigating these artifacts, which imply poorer measurement accuracy for the lowermost stratosphere (as expected from the error analysis in section 5).

Since the current 183-GHz ozone retrievals are not sensitive enough at 100 hPa, we are not advertising this level as a useful one for those retrievals. The main systematic effect to note is the existence of larger ozone values in earlier (not publicly released) MLS data versions, compared to the 205-GHz values, for middle to upper stratospheric heights. These differences were of the order of 10–15% (see Figure 15) in postlaunch retrievals (preversion 3 data). Although it has become clear that systematic error sources are much more likely for the 183 GHz ozone data (see section 5) and could, in principle, explain these differences, a full understanding of the actual sources of this discrepancy is not available yet. We also note that the 205-GHz ozone data have consistently given better comparisons with other data sets (see below) than the 183-GHz results. Uncertainties in sideband ratios and the 183-GHz radiometer pointing misalignment could, in principle, combine to account for a large portion of this effect. An independent analysis of radiometer pointing misalignments through the use of moon scan analyses [see Jarrot *et al.*, this issue] has





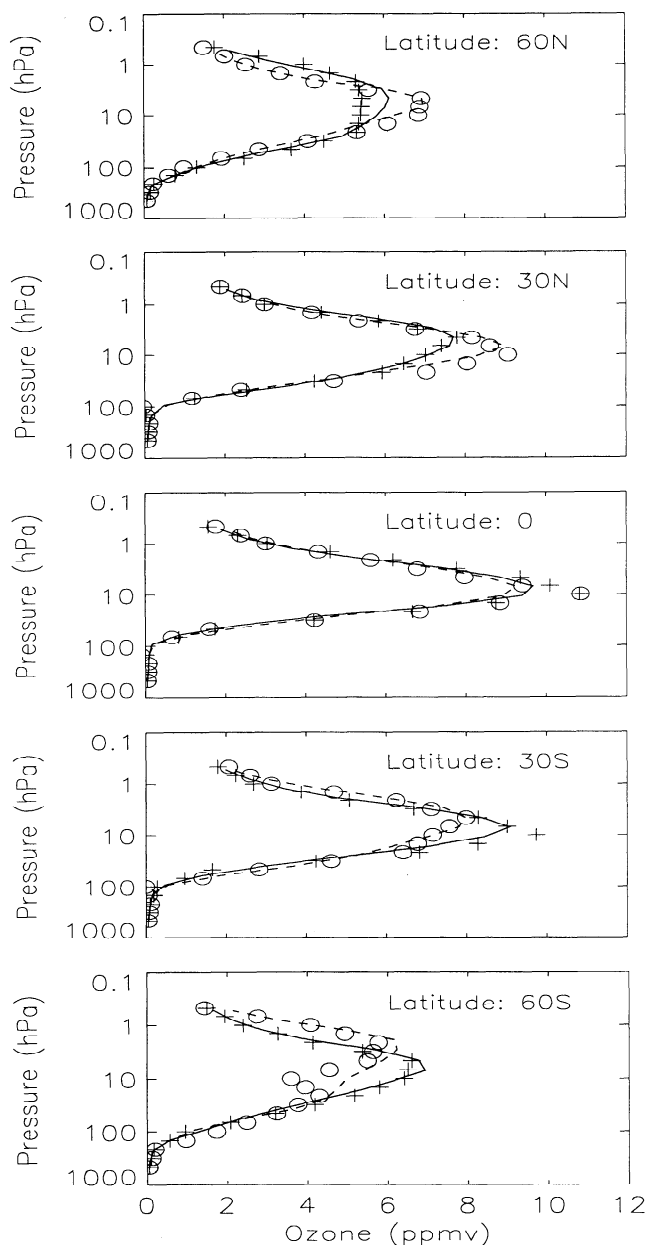
**Plate 4.** Zonally averaged diagnostic ( $\chi_{ma}^2$ ) as a function of latitude and time, for radiances in the 205-GHz radiometer ozone band (top), and the 183-GHz ozone band (bottom). Left panels are for the first year of UARS MLS data, and right panels are for the second year (no data beyond mid-April from the 183-GHz radiometer). Color bars on the right give the scale for  $\chi_{ma}^2$  values.

led to the conclusion that a shift (possibly incurred during launch) exists in comparison to the prelaunch alignment determination. The MLS Version 3 data include a shift consistent with these findings but not quite so large as the final result obtained from the moon scan analyses (possibly because of compensating sideband ratio errors). Figure 15 demonstrates the better agreement currently found between the two ozone retrievals, using a semiempirical FOV elevation adjustment to basically match the average ozone 205-GHz and 183-GHz Version 3 retrievals. We stress that relative variations in 183-GHz ozone data should be emphasized rather than

absolute values (for which the 205-GHz data are recommended). A reevaluation of the parameters which can affect the MLS ozone data is in progress, in light also of the newer O<sub>2</sub> spectroscopic data, which has affected the retrieved tangent pressures by  $\sim 4\%$  in more recent analyses (see section 5 and *Fishbein et al.* [this issue]). A brief update concerning this topic is provided in section 8.

## 5. Estimated Uncertainties

In this section, an estimated error budget is formulated. Comparisons with other data sets can help detect



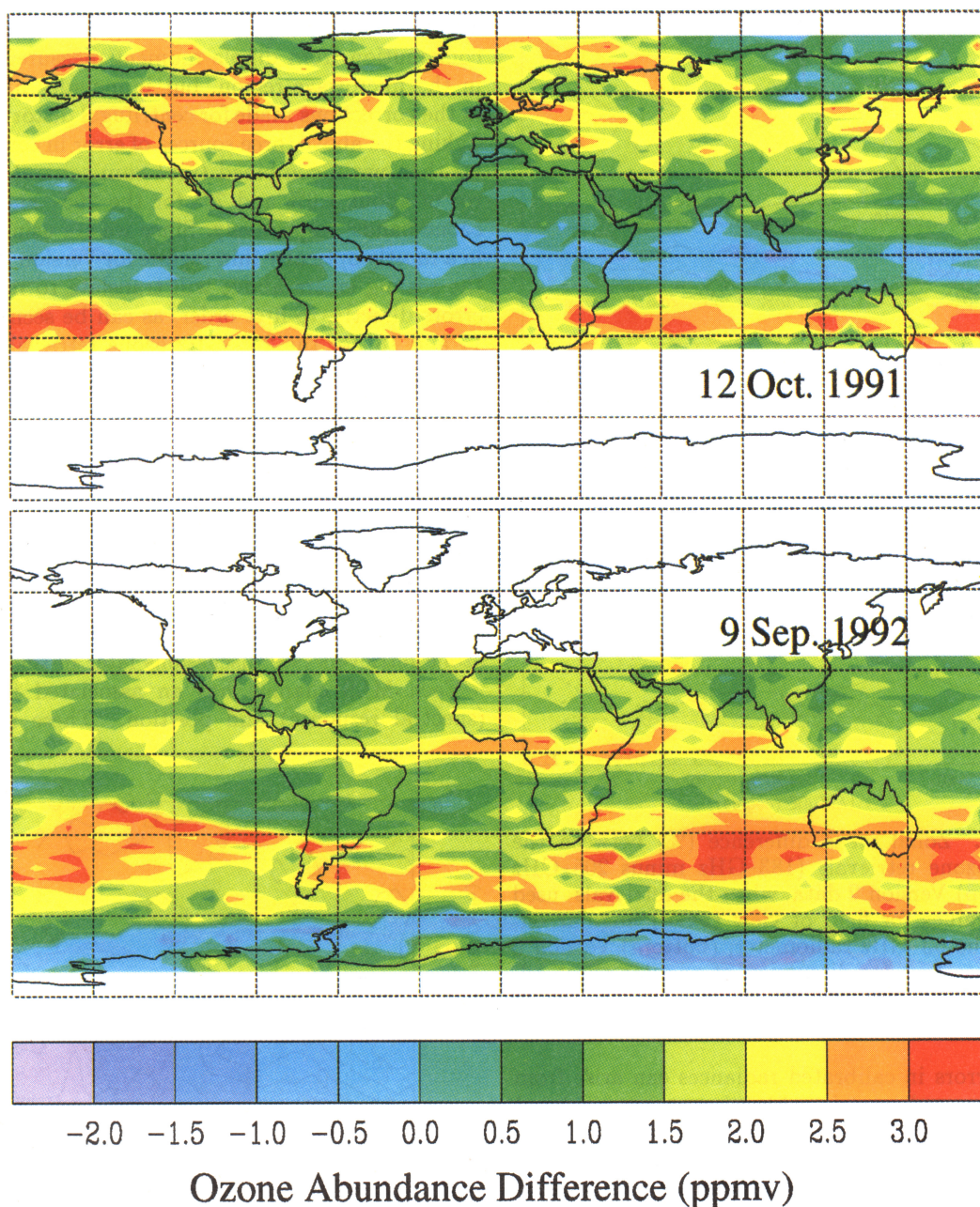
**Figure 14.** MLS 205-GHz ozone profiles versus climatological profiles for January and July. The climatological data (see text) are shown for January (solid line) and July (dashed line) at the various latitudes shown in the five panels (60°N, 30°N, 0°, 30°S, and 60°S, top to bottom). MLS ozone values are given by pluses for January, and open circles for July, at the same latitudes (zonal means over a 5°-wide bin centered at the above latitudes); four days of MLS data in mid-January and mid-July 1993 were used here.

biases, and we will see in the next section how consistent those analyses are with the uncertainties presented here.

The error sources which can impact MLS ozone retrievals can arise for the following reasons: (1) radiance noise; (2) radiance scaling error (includes radiometric, sideband ratio, and line strength errors); (3) error in filter shapes; (4) error in FOV direction (relative to the 63-GHz radiometer FOV); (5) error in FOV shape

(includes spectral dependence); (6) error in ozone line width; (7) errors from retrieval numerics; (8) error contribution from a priori; (9) error in  $P_{\text{tan}}$ ; (10) error in atmospheric temperature; (11) error in dry air continuum; (12) error in knowledge of  $H_2O$ ; (13) error in knowledge of  $HNO_3$ ; (14) error in knowledge of  $N_2O$ ; (15) error in knowledge of  $SO_2$ . The last three error sources were only considered in the analysis of 205-GHz ozone. Other sources of error exist but are either implicitly included in the above list or considered to be negligible (see below). The above error sources lead to mostly systematic errors, and the MLS ozone sensitivity to these factors is studied, primarily via a series of tests for one day's retrievals. In principle, the error analysis method of Rodgers [1990] could be applied here instead of sensitivity tests, with equivalent results (we did use this approach for the measurement noise and smoothing or a priori error contributions); however, issues like latitude dependence of errors and errors in forward model parameters can sometimes be more easily studied using the actual retrieval algorithms and their sensitivity.

First a comment is worthwhile, regarding the uncertainties listed in the Version 3 MLS data files. In general, the estimated rms uncertainties in these files are somewhat larger than the actual atmospheric rms variability, particularly in the lowermost altitude range. Figure 16 is an example of a relatively quiet day (from an atmospheric variability point of view) and shows the ratio of rms variability (about the zonal means) to estimated rms uncertainties (from Version 3 ozone results for 205-GHz radiometer data), contoured versus latitude and pressure. Ratios smaller than unity can occur in regions of poor measurement sensitivity, as occurs near the tropopause (especially for the 183-GHz ozone), where the a priori constraint can artificially reduce the variability relative to the generally very conservative a priori uncertainty. Also, some error sources included in the retrieval code are not random in nature (e.g., part of the a priori tangent pressure estimated error arising from pointing knowledge uncertainty and its impact on ozone). Below we will compare the uncertainties from the MLS data files to the random and systematic error estimates derived below. We now turn to a discussion of the various error sources listed above. Resulting error estimates are given in Figures 17 and 18 for the 205- and 183-GHz radiometer data, respectively. Although plots cover the range 100 to 0.1 hPa, we caution that the recommended vertical range for useful scientific studies needs to be taken into account. Based on increasingly poor measurement sensitivity in the Version 3 data files and the error analyses (given below), 205-GHz ozone data analyses for altitudes above 0.46 hPa or below 46 hPa are not advised, nor are those for 183-GHz data at altitudes above 0.046 hPa or below 46 hPa. Some information is contained at the limiting levels indicated above (and even at Level 2 pressures above and below these), but the full capability of the measurements will need to be exploited better in a future MLS data version. Error contributions near and beyond the limits stated above will change somewhat

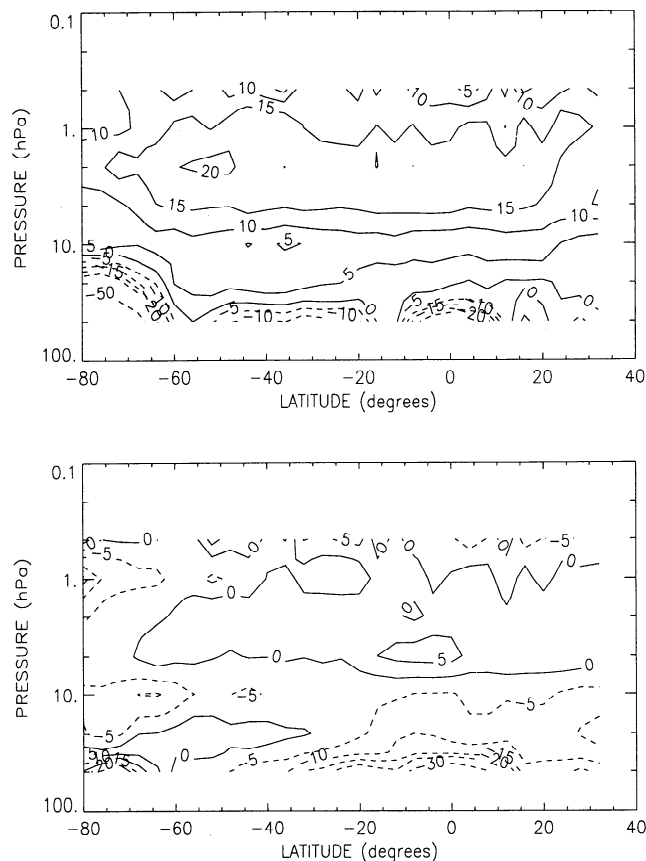


**Plate 5.** Mapped field of the MLS-retrieved ozone abundances at 46 hPa minus those at 100 hPa; blue and purple colors indicate a negative difference, i.e., a retrieval artifact (“bulge” at 100 hPa), if sustained over a large area, not just a noise effect. These tend to occur at polar and equatorial latitudes. (Top) North-viewing conditions on October 12, 1991, and (bottom) South-viewing conditions on September 12, 1992.

with such new software. For example, particularly for 183-GHz ozone data in the lowermost stratosphere, a priori error contribution will go down, but other error sources in this region are likely to go up because of their artificial “damping” by the a priori weighting (i.e., Figure 18 characteristics in the lowermost stratosphere will change).

Radiance noise determines the precision (repeatability) of the retrieved profiles. Precision estimates based on the measurement noise contribution (calculated via the method discussed by Rodgers [1990] are shown in Figures 17 and 18. These values are close to but (as

expected) generally slightly lower than those obtained from an empirical estimate of precision, i.e., based on observed variability during several summer (“quiet”) days near the orbit turnaround tangent points (latitudes of 34°N or 34°S), where the densest sampling occurs, and several tropical data sets (where actual atmospheric variability is also expected to be near minimum). We have kept the theoretical estimates of precision as probably the better indicator of true precision (this could only be checked exactly if the same atmospheric parcel was monitored for many measurements, and if atmospheric variability was negligible).

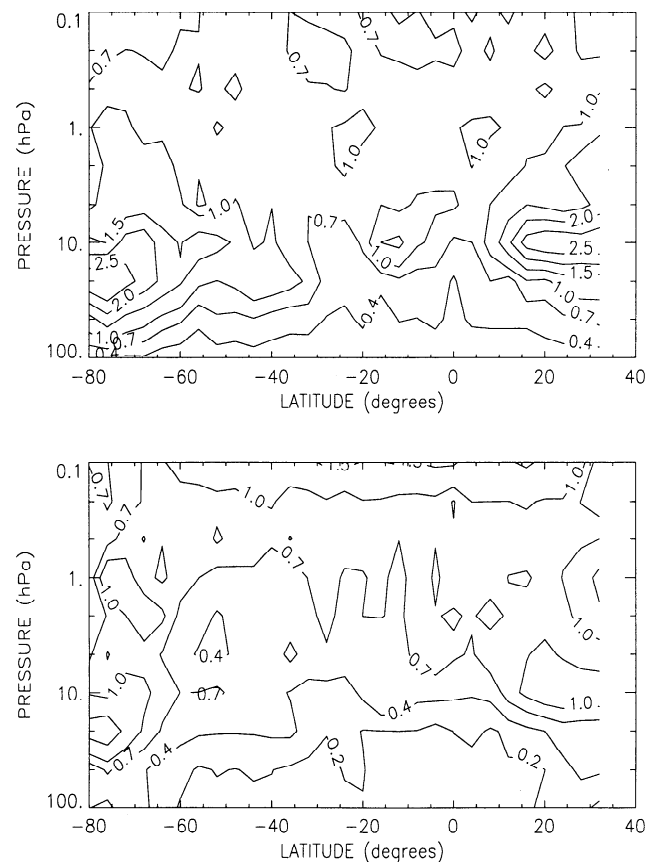


**Figure 15.** Zonal mean difference (%) between the two MLS ozone retrievals (183-GHz minus 205-GHz ozone). (Top) Version 2 data, when the retrievals used prelaunch values for field of view (FOV) angular offset versus the 63-GHz radiometer; (bottom) Version 3 retrievals (see text for discussion of angular offset adjustment).

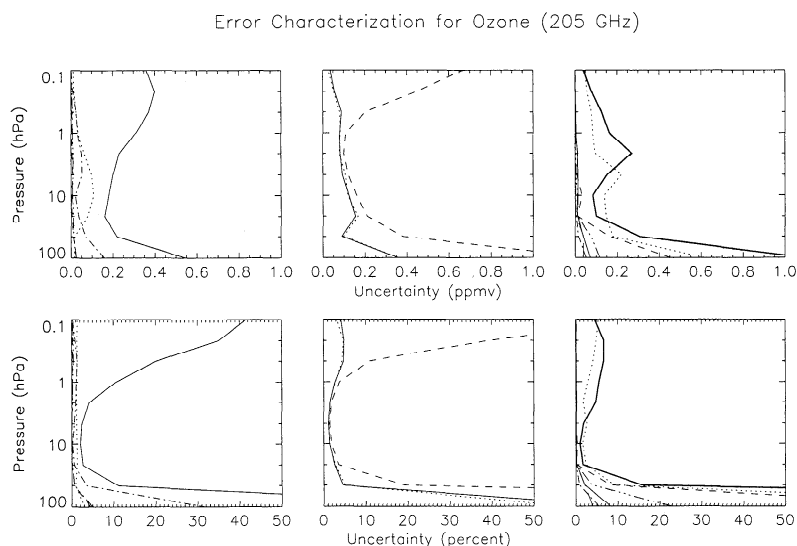
Scaling errors in calibrated radiances can arise from three sources: radiometric calibration errors, sideband ratio errors, and spectroscopic errors in line strengths. The first two sources of error are discussed by *Jarnot et al.* [this issue]. Based on this reference, we use a systematic error (“one sigma type”) of 0.6% for the radiometric calibration of the 205-GHz and 183-GHz radiometers, which is assumed to correspond to about one third of the worst-case error expected; this error reflects mostly uncertainties in the characterization of losses through the MLS antenna and switching mirror. Note that a spectrally flat radiance offset across the band(s) is taken out by the retrieval software, which uses only spectral contrast to retrieve mixing ratio values. Radiances from the two sidebands are combined to yield total radiances for each ozone band. The relative weighting of each sideband is described by the sideband ratio values [see *Jarnot et al.*, this issue], determined before launch. Based on the above reference, sideband ratio errors can lead to likely (one third of worst case) radiance errors of 0.6% for the 205-GHz ozone band and 7% for the much poorer characterization of the 183-GHz ozone band. Finally, a systematic line strength error of 0.5% is used for the ozone lines considered here (H. Pickett, private

communication, 1994); this is larger than the intrinsic contribution from dipole moment measurement errors in the microwave region, but it includes uncertainties in the corrections made for centrifugal distortion effects. Taking the above three sources of error in consideration, we then use a combined (root sum square) scaling error of about 1.0% and 7% for the 205- and 183-GHz ozone bands, respectively. Since we are using radiances in a mostly optically thin regime for Version 3 data files, the scaling errors above will translate to mixing ratio errors directly, to first order, as can be seen in Figures 17 and 18; for the 205-GHz ozone retrievals, radiance scaling uncertainties lead to slightly more than 1% error, whereas the 7% radiance scaling error for the 183-GHz band can produce 8 to 10% errors in ozone for pressures less than 22 hPa, with increasing (nonlinear) effects at higher pressures. The 183-GHz ozone error budget is largely dominated by this potential radiance scaling error (arising from the poorer characterization of sideband ratios). Ozone abundances obtained from the 205-GHz radiometer should give a better indication of the actual systematic error to expect in the 183-GHz ozone retrievals (see discussions later in this paper).

Each MLS channel has an associated filter shape (spectral response) and position. There is a poten-



**Figure 16.** Rms variability about zonal means divided by estimated uncertainty (from MLS Version 3 data files), for November 28, 1992 (a day with minimal variability), for 205-GHz ozone (top) and 183-GHz ozone (bottom).

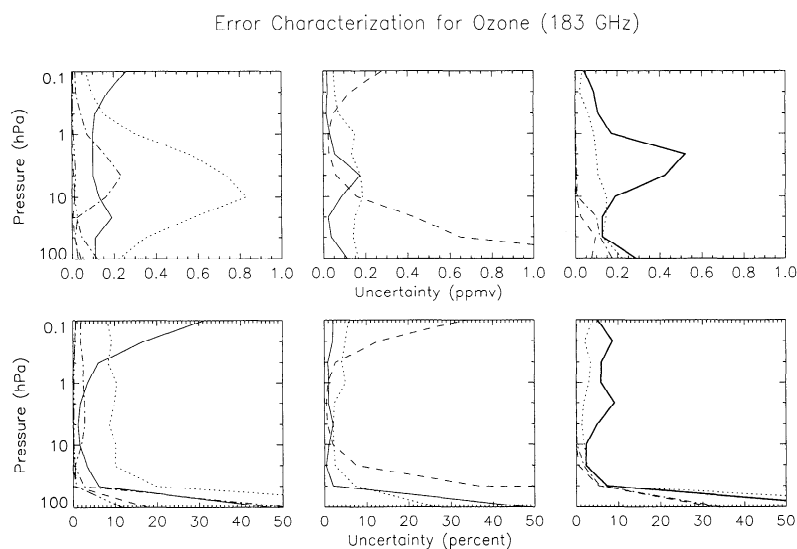


**Figure 17.** Error characterization for the MLS 205-GHz ozone data. Rms uncertainty estimates are given for the various error sources listed in Table 1. Top panels give uncertainty in parts per million by volume, and bottom panels give the values as a percentage; results are generally averaged over all latitudes based on sensitivity tests for a full day of MLS retrievals (see text for details). (Left): Uncertainties from radiance noise (solid line), and systematic errors in radiance scaling (dotted line), filter shapes (dashed line), essentially negligible, only seen as 5% effect at 100 hPa, FOV direction (dashed-dotted), and FOV shape (dashed-dotted-dotted). (Middle): Uncertainties from ozone line width (solid line), retrieval numerics (dotted line), and smoothing error contribution (dashed line). (Right): Uncertainties from systematic error in knowledge of  $P_{\text{tan}}$  (thick solid line), temperature (dotted line), dry air continuum (dashed line), H<sub>2</sub>O (dashed-dotted), HNO<sub>3</sub> (dashed-dotted-dotted), N<sub>2</sub>O (long-dashed line), and SO<sub>2</sub> (thin line).

tial source of error in the knowledge of filter shape [see *Jarnot et al.*, this issue]. Following the above reference, we have used an uncertainty of 0.03% per MHz slope on the existing filter transmission functions as a worst case; this bias was applied for all channels on one side of the ozone line and with a different sign on the other side, as a worst case scenario. Resulting errors are essentially negligible, as exemplified in Figures 17 and 18,

where the plotted rms-type errors (worst case divided by 3) are barely visible in the lowermost stratosphere.

Errors in field of view (FOV) direction have to do with the uncertainty in knowledge of the true pointing direction of each radiometer. In the case of ozone we are interested in possible errors arising from any misalignment of the 205-GHz or 183-GHz radiometer FOV with respect to the 63-GHz FOV (errors in absolute pointing



**Figure 18.** Same as Figure 17 but for ozone from 183-GHz band data. The last three error sources (from HNO<sub>3</sub>, N<sub>2</sub>O, and SO<sub>2</sub>) in Figure 17 are not present for 183-GHz ozone.

of the 63-GHz FOV are accounted for below as possible systematic errors in tangent pressure). Although preliminary postlaunch moon-viewing calibration data gave no indication of a need to reconsider the alignment of the 205-GHz radiometer (to within the prelaunch errors), the 183-GHz radiometer data indicate the need for an alignment adjustment from the prelaunch value [see *Jarnot et al.*, this issue]. Changes in the software parameters producing Version 3 data were made to accommodate a possible misalignment consistent with the moon calibration data as well as the observed differences in ozone between the independent radiometer data. The MLS Version 3 data used a misalignment value of  $0.006^\circ$  (about 290 m in tangent height), somewhat less than the moon-derived result of  $0.011^\circ$  (finalized only after the software changes for Version 3 data production), albeit consistent within the errors of the alignment determination. Elevation alignment errors of  $0.0016$  and  $0.012^\circ$ , for the 205- and 183-GHz radiometers, respectively, were used as the basis for our estimates of profile errors arising from remaining (worst case) misalignments in FOV direction; the first number corresponds to prelaunch (worst case) knowledge for the 205-GHz radiometer data, while the second number reflects the postlaunch uncertainty based on moon calibration tests for the 183-GHz radiometer, since independent evidence on ozone abundances indicate that there is reason to place more confidence in the postlaunch numbers for the 183-GHz radiometer. In fact, the 183-GHz uncertainty (in relative FOV direction) used here is a conservative number, since we have added the (“3 sigma”) uncertainty ( $0.007^\circ$ ) from moon scan analyses [see *Jarnot et al.*, this issue] to the possible alignment change required ( $0.005^\circ$ ) to best fit the moon scan results alone (not the 205-GHz ozone results). Results in Figures 17 and 18 are based on these worst-case sensitivity tests and a factor of 3 reduction to provide rms-type uncertainties. The larger uncertainty for the 183-GHz radiometer FOV gives rise to the more significant potential systematic errors (a few %) seen in Figure 18.

Errors in FOV shape were also considered, by assuming that an error in beam width (radiometer dependent) can modify the retrievals and so can an error in the pattern’s sidelobe levels. For the 205-GHz radiometer, based on *Jarnot et al.* [this issue], a worst-case beam width error of  $0.003^\circ$  was assumed. The spectral dependence of the field of view is less than the estimated accuracy in FOV beam width ( $0.003^\circ$ ), as mentioned by *Jarnot et al.* [1995]. For the 183-GHz radiometer, somewhat larger errors are used, based on the fact that the postlaunch determination of FOV misalignment for this radiometer would lead one to suspect a corresponding error in FOV shape as well (i.e., different from the measured shape, which assumed a different alignment). Using an estimate of the likely change in FOV shape from the worst-case misalignment in 183-GHz radiometer FOV ( $0.018^\circ$ ), we have used an error in beam width of  $0.005^\circ$  as a worst-case possibility. The resulting ozone rms errors (worst case divided by 3) shown in Figures 17 and 18 do not play a major

role compared to other systematic error sources. Errors in antenna sidelobe knowledge are considered negligible for ozone retrievals in the stratosphere, given the small (1%) amount of lower atmospheric radiance contribution from the sidelobes and its even smaller spectral contribution. The relative error contribution from sidelobe level uncertainties should be a maximum when the antenna is pointing near 60–70 km, and the lower sidelobes are receiving strong signals from the troposphere (with weaker signals arising from the tangent point).

Spectroscopy errors can clearly lead to retrieved profile errors. Errors in line strength have been included above as part of radiance scaling errors. Line positions are known extremely accurately at microwave wavelengths and thus do not represent a significant error source. A related error could arise from imperfect knowledge of the Doppler shift of the emitted radiation, caused by line of sight velocity effects. Since the spacecraft and Earth velocity components along the line of sight are quite well known and are accounted for in the retrieval algorithms, atmospheric wind will constitute the largest error source, with maximum effect in the lower mesosphere (and for channels adjacent to the center channel). For a conservative line of sight velocity error of 50 m/s the ozone radiances for the 205-GHz radiometer will be negligibly affected (less than a 0.05 K effect). For the 183-GHz ozone line, a 1–2% (0.2 K) effect on some radiances is possible, but this is a negligible effect in the stratosphere, and we have already mentioned significantly larger error sources for these retrievals. To include possible errors in linewidths, a 3% error in the broadening function was used to estimate systematic errors in profiles arising from this source, based on the spectroscopic work of *Oh and Cohen* [1992], who quote a 3% accuracy value. Corresponding ozone uncertainties (treated here conservatively as “one sigma” values) are given in Figures 17 and 18.

Errors arising from retrieval numerics refer to the differences between the mixing ratio profiles used to create simulated noise-free radiances, and the subsequently retrieved ozone profiles, keeping other parameters (e.g., tangent pressure and temperature) set to the “true” (known) values. This error source is fairly small (see Figures 17 and 18).

“The smoothing error,” as expressed by the null space error term described by *Rodgers* [1990] and discussed further by *Marks and Rodgers* [1993] is included in the middle panels of Figures 17 and 18. As mentioned earlier for the averaging kernel calculation which enters into this error term, results will be somewhat different if a finer resolution grid for the true profiles is assumed. Mainly, the smoothing error could be somewhat larger in the region of good measurement sensitivity. This is because the smoothing error includes both the effects of finite measurement resolution and a priori constraints, whereas Figures 17 and 18 show mainly the a priori error contribution. However, we note that if smoothing of correlative data is performed using the MLS averaging kernels, there is then no need to include a smoothing error contribution in the MLS-retrieved values. This

source of uncertainty is needed if one uses the MLS retrieval data as "point values" at each pressure level, which they really are not. As expected, the smoothing error is small in the region of good measurement sensitivity (10 to 1 hPa in particular) but rises in the in the mesosphere and lower stratosphere; 205-GHz ozone data are dominated by a priori contribution in most of the mesosphere, where 183-GHz ozone data are more measurement sensitive, whereas the current 183-GHz ozone retrievals lose sensitivity below the 10-hPa altitude more quickly than the 205-GHz ozone values. If all the measurement channels were included (as planned in a future software version), the smoothing error contribution would be smaller than shown here, especially for the 183-GHz data near 100 hPa.

Errors in tangent pressure can clearly give rise to errors in mixing ratios (which are based on radiances at the retrieved tangent pressures). A possible systematic error in  $P_{\text{tan}}$  of about 6% [see *Fishbein et al.*, this issue] is assumed here, corresponding to about 300 m in tangent height. This potential error can have a significant impact on ozone (5 to 15 % for altitudes at and above 46 hPa) and arises primarily from possible errors in the O<sub>2</sub> spectroscopic database. Indeed, postVersion 3 MLS data updates will include the latest recommended spectroscopic database by *Liebe et al.* [1992], which leads to a 6% change in O<sub>2</sub> line width. A smaller (3%) error from this source may be more reasonable for updated MLS software, although other error sources can also have some impact on the tangent pressure determination [see *Fishbein et al.*, this issue].

Similarly, systematic biases in temperature can lead to biases in mixing ratios, since the radiances in the ozone band(s) depend somewhat on temperature; this is a linear function at microwave wavelengths, where the temperature dependence is much weaker than in the infrared or ultraviolet. Biases in temperature were taken to be 2 K for nonpolar latitudes and 5 K for latitudes poleward of 60°; these values are consistent with observed average differences between MLS and National Meteorological Center (NMC) temperatures (MLS giving lower results; see *Fishbein et al.* [this issue]). The effect of temperature biases was isolated by imposing these biases, while tangent pressure and other parameters were constrained to "truth." Corresponding rms changes in mixing ratios were then used to give the ozone systematic errors plotted here (see Figures 17 and 18). Typically, ozone uncertainties arising from such potential biases are of the order of 2-3 % and somewhat larger in the lowermost stratosphere; the 183-GHz results are slightly less sensitive to temperature than the 205-GHz results.

Error sources numbered 11 through 15 (above) deal with imperfect knowledge of emission features in the ozone band(s). The dry air continuum is a semiempirical contribution derived from the radiance data in wing channels of the 205-GHz nonozone-emission regions. Errors arising from imperfect knowledge of this continuum are obtained by using a "worst-case" scenario in the forward model, with no such continuum, and comparing retrieved profiles to the standard run.

Similarly, errors in other constituents such as HNO<sub>3</sub>, N<sub>2</sub>O, H<sub>2</sub>O, and SO<sub>2</sub> were considered, especially for the lower stratosphere. These error sources lead to profile errors primarily in the lower stratosphere. HNO<sub>3</sub> was not retrieved by MLS software until after Version 3 data were created, and here we will use HNO<sub>3</sub> errors appropriate to this data version. The differences between ozone retrievals using climatological assumptions for HNO<sub>3</sub> versus MLS-retrieved HNO<sub>3</sub> provide a basis for ozone errors arising from uncertain knowledge of HNO<sub>3</sub>. This error source should be reduced in future MLS data processing.

N<sub>2</sub>O is a contaminant of the ozone data near 205-GHz because of a line outside the ozone band which provides a (sloping) continuum in the ozone band, primarily in the lower stratosphere. Given the lack of enough spectral contrast for retrieving N<sub>2</sub>O, however, we assume climatological values, and errors in this assumption can lead to errors in ozone. A systematic bias of 20 % has been used here as the basis for the N<sub>2</sub>O uncertainty effect on ozone retrievals. The same has been done for sensitivity to H<sub>2</sub>O (this species also enters as a continuum effect in the ozone bands); the effect of water vapor comes mostly from below the tropopause, however, where large increases and variability can occur. Although MLS data contain information on water vapor slightly below the tropopause [*Read et al.*, 1994], this is not part of routine MLS Version 3 processing and was not used (as a constraint) in the Version 3 ozone retrievals. The uncertainty results for poor knowledge of these species are displayed in Figures 17 and 18. It may be that certain times and places are more subject to these types of errors, and the values used here are only a guide. Generally, these effects are to be considered smaller than the inexact knowledge of tangent pressure (and temperature, to a lesser degree).

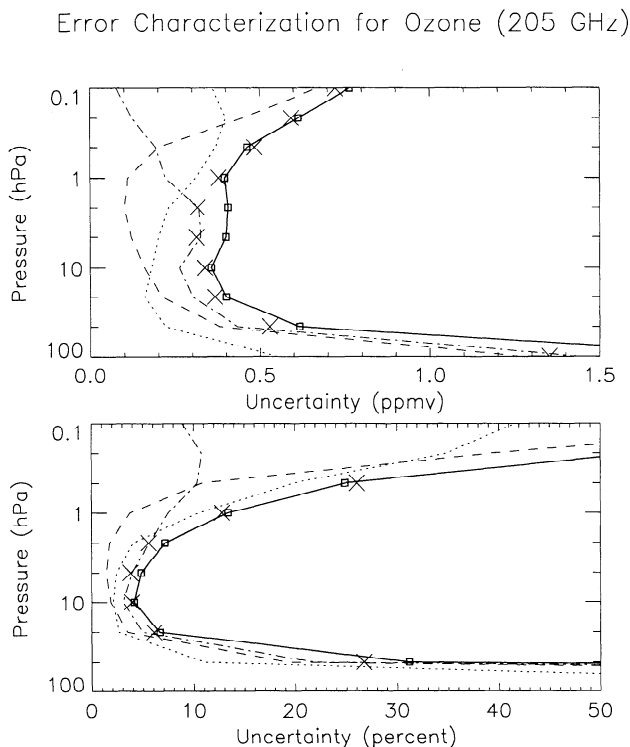
Finally, the effect of SO<sub>2</sub> should have a small impact on ozone (at 205 GHz) only during enhanced conditions (e.g., following the Mount Pinatubo eruption). To illustrate this here, we have used conditions of enhanced SO<sub>2</sub>, at the 1 part per billion (ppbv) level in the lower stratosphere (more than 10 times background but 10 times less than the highest Pinatubo effect observed by MLS, as discussed by *Read et al.* [1993]). This type of SO<sub>2</sub> "contamination" can give rise to 5% ozone errors in the lowermost stratosphere, similar to the effects of H<sub>2</sub>O and N<sub>2</sub>O mentioned above, in the 46- to 100-hPa range. However, under background conditions, such errors will not appear. A future retrieval scheme will account for the amounts retrieved by MLS, especially under enhanced conditions.

We see from the right-hand panels of Figures 17 and 18 that uncertain knowledge of certain atmospheric parameters can have a significant impact on ozone accuracy, especially at the lowermost altitudes. Most of these factors play a minimal role, however, for altitudes above 46 hPa, and tangent pressure uncertainties tend to dominate other effects at most altitudes. Errors in minor constituents O<sup>18</sup>OO and HO<sub>2</sub> are negligible because of the small signal strengths arising from these molecules; the O<sup>18</sup>OO mixing ratio should be

well enough constrained from the ozone retrieval values, based on the expected isotopic ratio.

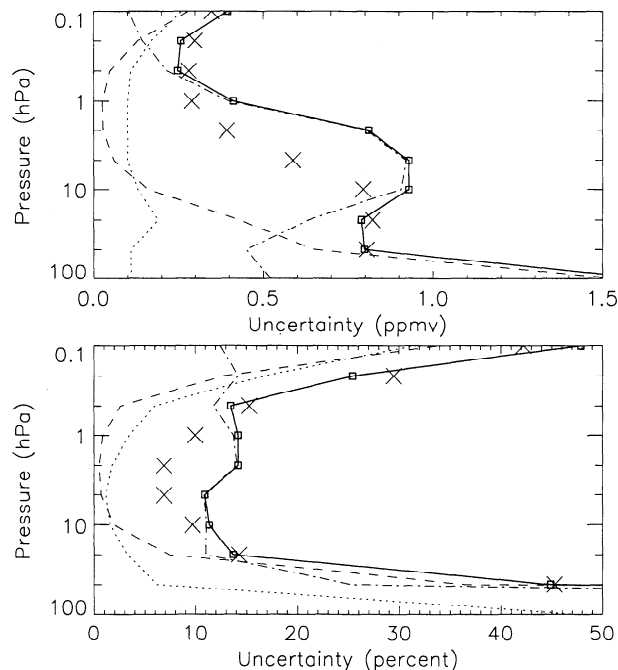
Finally, there is a small residual spectral baseline in the MLS spectra, after an empirical (postlaunch) set of channel-dependent offsets of the order of 0.1 K has been removed from the spectra, by using data at the highest tangent altitudes [Jarnot *et al.*, this issue]. Variations in this residual baseline (as well as small average changes determined since the Version 3 data were processed) can be used to ascertain the effect of this error source. Since these variations are of the order of a few hundredths of a degree or less, typically, this will have minimal (much less than 1%) impact on ozone retrievals, where signals are of the order of tens of degrees; other error contributions make this source of error negligible. A scan-dependent spectral baseline would not be detectable in normal operations, but analysis of radiances taken during satellite roll maneuvers shows this is insignificant (for individual retrievals).

Figures 19 and 20 give the total estimated uncertainties (random, systematic, and smoothing error contributions, along with the root sum square of these as total uncertainty) for the 205-GHz and 183-GHz retrievals, respectively. We can see from these figures that the 205-



**Figure 19.** Total estimated uncertainty for the 205-GHz radiometer ozone. Random (dotted line), systematic (dashed-dotted line), and smoothing (a priori) error contributions (dashed line), along with total (rss) uncertainties (solid lines connecting squares) are plotted as a function of pressure. Also, typical (global rms) uncertainty values given in MLS Version 3 data files are shown as crosses (see text for discussion). (Top) Values in parts per million by volume and (bottom) in percent (of global rms profile for September 17, 1992).

Error Characterization for Ozone (183 GHz)



**Figure 20.** Same as Figure 19 but for the 183-GHz ozone.

GHz ozone uncertainty is not dominated by the systematic effects (rms estimate of 10 to 15 %) which account for the main part of the 183-GHz error budget (in the 1 to 20-hPa region). Ozone results from the 183-GHz band will be most useful for mesospheric studies, especially those dealing primarily with relative changes (e.g., diurnal variation analyses as in the work of Ricaud *et al.* [this issue]). The random (measurement) noise component plays a major role for 205-GHz ozone data from 0.5 to 10 hPa, with (rms) systematic effects possible also at the 2 to 9 % level. At 46 and 100 hPa the a priori and systematic error contributions will dominate; this is evident in some of the comparisons discussed in the next section, as well as in the artifacts mentioned earlier, where averaging the profiles still leaves a systematic effect, e.g., the yaw cycle dependence at 100 hPa. The estimated uncertainties derived by the MLS software algorithms are also indicated in Figures 19 and 20, for comparison; these values are generally somewhat larger than the estimated precision in the profiles, from a few percent larger in the upper stratosphere to a factor of more than 2 at 100 hPa. Middle-to lower stratospheric Levels 2 and 3 profile uncertainties should therefore be looked at as being close to the total rms uncertainty for ozone results at 205 GHz and as a lower bound to the total (rms) uncertainty for the 183-GHz ozone retrievals. Ideally, statistical quantities such as the estimated errors in average ozone (over a latitude region and/or a period of time) should also be handled with these facts in mind, namely, that only the random part of the total uncertainty can be reduced by the averaging process; in principle, the a priori error contribution



can also be removed [e.g., Connor *et al.*, 1994]. Using in large part the figures above, we will summarize the estimated precision and accuracy values in tabular form in section 7.

We note that the optimum use of all channels (especially for 183-GHz ozone data) and a decrease in the radiance error inflator factor (see section 3), which is likely to occur in the future, will lead to a reduction in estimated precision and a priori error contribution. Tests with this kind of treatment suggest that the main change for the 205-GHz data would be a precision at 100 hPa closer to 0.25 ppmv and a value of 0.1 ppmv for a priori error contribution at pressures between 100 and 1 hPa. For the 183-GHz ozone data the a priori error contribution would be significantly less than 0.1 ppmv from 1 to 100 hPa, and the precision would still be  $\sim 0.1$  ppmv for this region. In addition to this, systematic errors may not be as large as these estimates, which are not a definite statement about what biases actually exist. In fact, radiance residuals mapped onto parameter space lead us to believe that this "residual error" may typically be of the order of 0.2 ppmv for the 205-GHz ozone stratospheric data (using improved software algorithms); this is smaller than the systematic error estimate of Figure 19 in the lower stratosphere, although this type of residual error can only be looked at as a minimum systematic error (some errors, such as a line strength error, would not show up in the residuals). For ozone data from the 183-GHz band, however, residual errors in the lower stratosphere (even with an improved iterative retrieval) appear to be of the order of 0.5 ppmv or more, and more work will be needed to understand the sources of systematic errors (and reduce them). Nevertheless, improved MLS measurements of 100-hPa ozone mixing ratios are likely in the future.

## 6. Comparisons With Other Data Sets

In this section, comparisons between MLS ozone (205-GHz data) and other data sets are made. This should, in principle, give results which are compatible with the estimated accuracies given in section 5. The correlative data sets used here have a finer vertical resolution than the MLS data. Comparisons shown here use a simple interpolation of the correlative data onto the MLS retrieval grid. We have investigated to some extent possible quantitative effects introduced by the different vertical resolutions of these instruments; smoothing of the correlative data sets has been performed (in tests not shown here, for brevity) via a least squares fit method as well as the (more appropriate) convolution with the MLS averaging kernels (as done by Connor *et al.* [1994]). We feel that more work is needed to fully cover this topic and its implications (including subtle issues on the averaging kernel calculation; see section 3) and therefore choose to devote minimal space here on this subject. One would expect that if enough profiles are averaged, smoothing effects will be largely taken care of, even in the simple (but often used) "point-by-point" comparison method presented below. We gener-

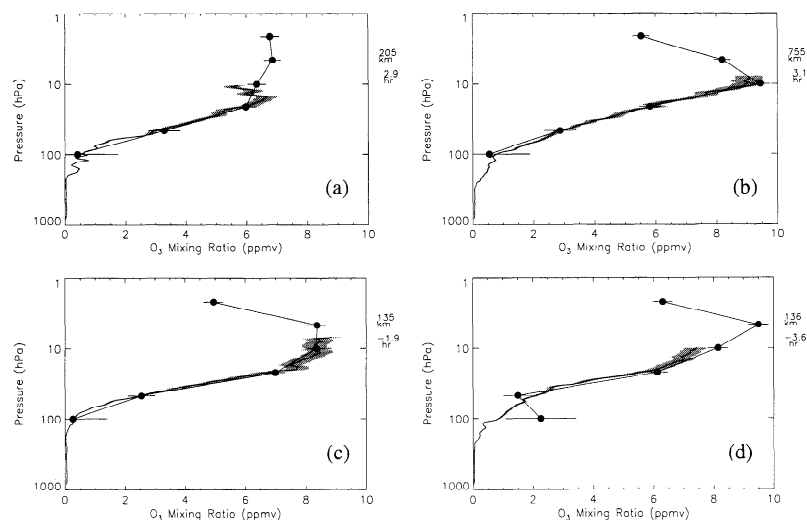
ally see no significant improvement in the comparisons when "smoothing" of correlative data is applied, and the overall results are similar (within 5 to 10 %), with no clear bias; a possible improvement in the tropics is noted below.

### Comparisons With Ozonesonde Data

Comparisons are made between MLS 205-GHz ozone and ozonesonde data from selected sites, in the 100- to 10-hPa range. The ozonesonde data used here generally include about a year of measurements and cover a range of latitudes: Boulder (40°N, 254.7°E), Hilo (19.4°N, 205.0°E), Ascension Island (8.0°S, 345.7°E), Brazzaville (4.3°S, 15.0°E), Gardermoen (60.1°N, 11.0°E), and McMurdo (77.5°S, 166.4°E). A search for possible biases in the MLS data set is one goal of these analyses, assuming that the data used as comparison are sufficiently accurate; we think this is the case but the "true" atmosphere is difficult to characterize at the sub-5% level of accuracy, and much work is required to prove that such a goal can be (or has been) met. As a guide, the error bar on the ozonesonde data presented here is taken to be 5% of the ozone abundance, which is probably somewhat of an underestimate, particularly at 10 hPa, based on earlier analyses relating to this measurement technique [Barnes *et al.*, 1985; Hilsenrath *et al.*, 1986]. Indeed, this "canonical" number may apply to precision (possibly as an upper bound) as well as accuracy (separately), but we will consider enough profiles in the average comparisons below that the uncertainty in the mean will be dominated by the absolute knowledge (accuracy); more recent information on measurement uncertainties for ozonesonde (and lidar) data can be found in intercomparison results by Beekmann *et al.* [1994].

**Boulder site.** The fine resolution ozonesonde data taken at varying time and space "locations" with respect to the coarser MLS profiles lend themselves better to statistical analyses, rather than individual comparisons. However, for Boulder, we present a few examples of individual profile comparisons (see Figure 21), one for each season in 1992. Changes as a function of time are similar for both sets of data (for example, the spring maximum is observed in Figure 21b). We have deliberately chosen to show in Figure 21d a poor comparison at 100 hPa, where the Version 3 MLS value significantly overestimates the ozonesonde value.

A full year (1992) time series comparison for all of the coincidences between 1992 Boulder sonde and MLS profiles is given in Plate 6 for the four MLS retrieval surfaces (10, 22, 46, and 100 hPa) within the ozonesonde stratospheric altitude range. At 10 hPa, ozonesonde data are generally considered less reliable than at the higher pressures; however, the cyclic annual ozone variations at this level are observed to be similar in both data sets. The same appears to hold for the 22- and 46-hPa levels, where there is good tracking of the more complex temporal variations in these data. At 100 hPa the MLS Version 3 values are not very useful, given the size of the estimated uncertainties, and a significant



**Figure 21.** Individual profile comparisons between MLS 205-GHz ozone and ozonesonde data from Boulder during 1992. Data were taken on the following dates: (a) January 3, (b) April 17, (c) July 29, and (d) October 8. Examples of good correspondence between the two data sets are shown (Figures 21a through 21c), as well as an example of an unresolved problem in MLS retrievals at 100 hPa (Figure 21d). MLS data are connected solid circles with estimated uncertainties from the (Version 3) data files (see text); correlative sonde data are given by solid line, with a shaded uncertainty of 5% (see text). Distance (kilometers) and time difference (hours) between the MLS retrieved profile and the sonde data are indicated on the right-hand side of each panel.

comparison of the variations is not meaningful. However, the average values at this level agree quite well; this is illustrated in Figure 22, where average sonde and MLS profiles for the data sets shown in Plate 6 are displayed, along with panels of mean and rms differences (in parts per million by volume and percent) and other quantities discussed below. The mean differences at all (four) levels of interest are only a few percent, which is within the overall uncertainty (precision) of the average values obtained here (the size of these uncertainties is at most the full width of the squares used as symbols for the mean differences). Any remaining average differences would have to be attributed mainly to systematic errors in either or both data sets, although a component of this may come from the different vertical resolution of the instruments.

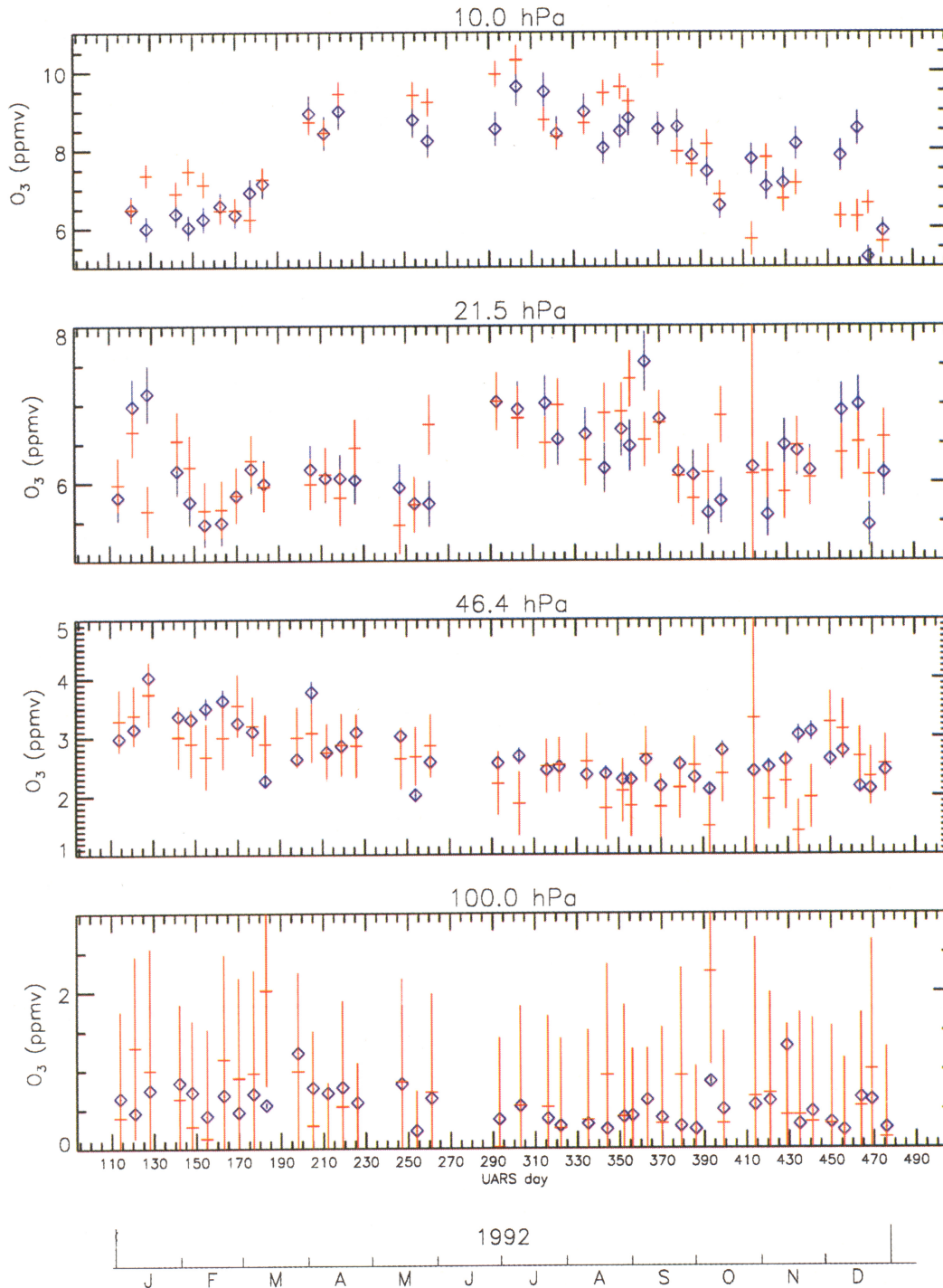
The standard deviation of the differences (between MLS and sonde data) is displayed in the bottom panels of Figure 22 (open circles) for comparison with the estimated rms precision of the differences (solid circles), i.e., the root sum square of the typical MLS and sonde precisions (see sections 5 and 7 for MLS ozone precision values). One would expect the standard deviation of the differences (which removes any average bias between the two data sets) to be equal to or larger than the rms precision estimate, and we see from Figure 22 that this is the case, but the standard deviations can be a factor of 2 larger than the rms precision. This could have several explanations: the possibly conservative 5% precision value for the sonde data (especially at 10 hPa), true atmospheric variability between the profiles sampled at noncoincident locations and times, vertical and horizontal resolution differences between MLS and sonde

profiles (fine scales not resolved by MLS), or other errors in the profile measurements. It is worth noting here that a large number of (smoothed) SAGE II ozone profiles have been compared to MLS ozone profiles [see *Cunnold et al.*, this issue (a)] and that the standard deviations of the differences between these data sets agree well with the rms precision estimates for the combined (difference) data. The other quantity shown in the bottom panels of Figure 22 is the rms difference between MLS and sonde profiles (this equals the root sum square of the average differences and the standard deviations of the differences); the rms differences obtained in this section are often dominated by the standard deviation of the differences (that is, the bias is small compared to the standard deviation). These rms differences could be viewed as an absolute worst-case total uncertainty in the MLS profiles.

**Hilo site.** Plots similar to Plate 6 and Figure 22, but for MLS ozone versus Hilo sonde data during 1992, are shown in Plate 7 and Figure 23. The agreement at 10 and 22 hPa is almost as good as for Boulder at those levels (near 5% mean difference, with MLS slightly high, and 5 to 10% rms difference). A larger percentage difference is observed in the lower stratosphere, with MLS ozone lower than the average sonde value at 46 hPa by almost 0.5 ppmv ( $\sim 20\%$ ) and larger than the sonde data at 100 hPa by  $\sim 0.2$  ppmv (which is a large percentage difference at the low values of ozone observed there). Excluding the 100 hPa level, the ozone variations measured by the sondes as a function of time at the various pressure surfaces are well reproduced by changes in the MLS ozone retrievals (with biases as mentioned above). Although the biases are somewhat larger than

O<sub>3</sub> Time Series: Boulder ozonesonde and MLS

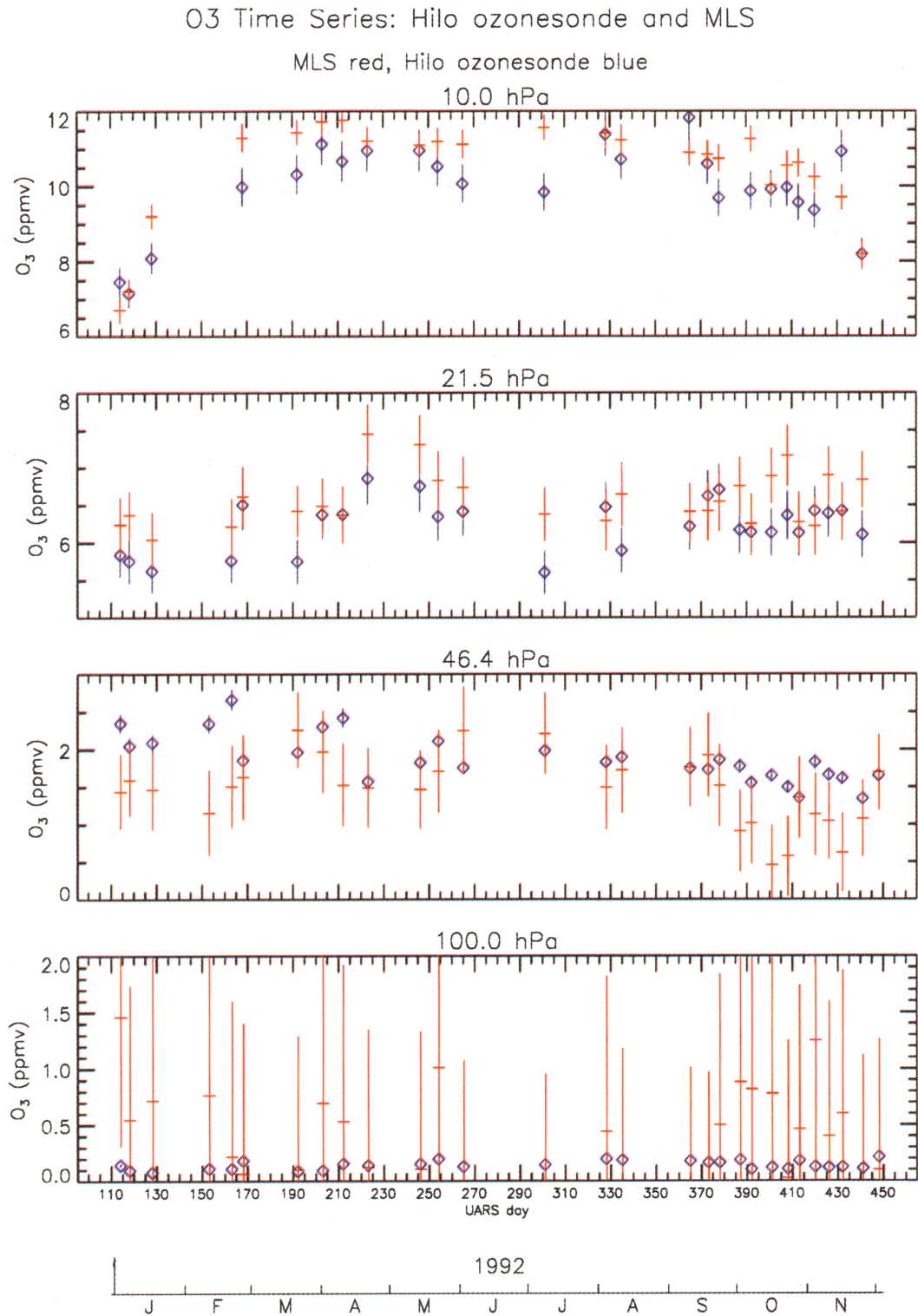
MLS red, Boulder ozonesonde blue



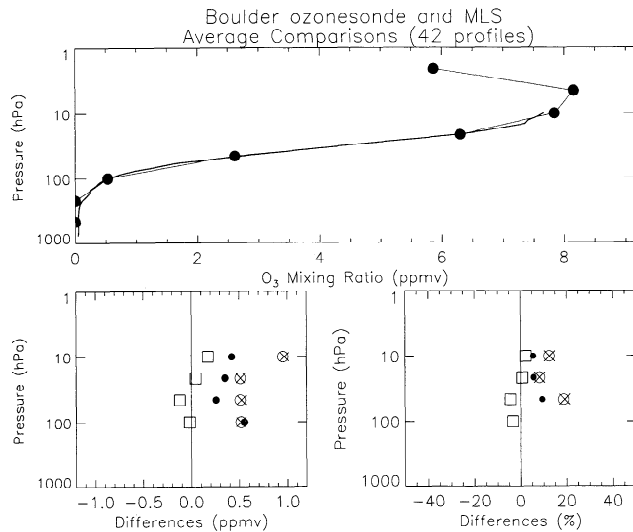
**Plate 6.** Time series comparison between MLS ozone mixing ratios (ppmv) at 100, 46, 22, and 10 hPa (bottom panel to top panel) and Boulder ozonesonde data during 1992 (42 coincident profiles total); MLS data (retrieved coefficients at the above pressures) are plus symbols (red) with estimated uncertainties (see text) and sonde data (with finer vertical resolution than MLS) are diamonds (blue) with estimated uncertainties (see text).

for the Boulder sonde data, the standard deviations of the differences (see Figure 23) are somewhat smaller, and the total (rms) differences are not very different from the values (in ppmv) shown in Figure 22.

**Ascension Island and Brazzaville sites.** The tropical ozonesonde data are of particular importance since the eruption of Mt. Pinatubo, and we examine next two data sets in the region just south of the equa-



**Plate 7.** Time series comparison between MLS ozone mixing ratios (ppmv) at 100, 46, 22, and 10 hPa (bottom panel to top panel) and Hilo ozonesonde data during 1992 (29 coincident profiles total); format is same as for Plate 6.

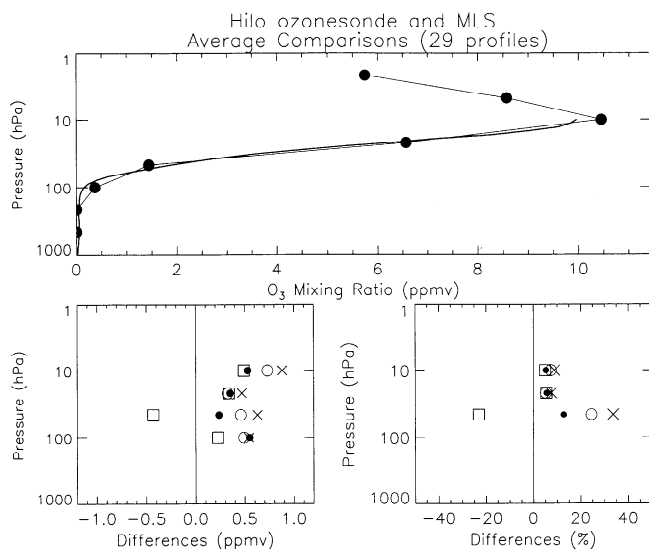


**Figure 22.** Statistics of comparisons between MLS ozone profiles and coincident Boulder ozonesonde data presented in Plate 6. (Top) Average MLS ozone profile (ppmv), solid circles connected by line, and sonde profile, thick line; (bottom left) average differences (ppmv) at the MLS retrieval grid points (100, 46, 22, and 10 hPa), squares, and rms differences (ppmv), crosses, along with the standard deviations of the differences, open circles, and the estimated rms precision of the differences, solid circles; (bottom right) same as in bottom left panel, but as a percentage of the mean sonde profile.

tor. Comparison plots are given in Plate 8 and Figure 24 for Ascension Island, and in Plate 9 and Figure 25 for Brazzaville. The results from the two sites, for about 1 year of data (October 1991 to roughly September 1992) give consistent mean differences with MLS ozone. A 5 to 10% systematic overestimate of the sonde ozone values exists in the MLS abundances at 10 and 22 hPa, while a  $\sim 20\%$  underestimate occurs at 46 hPa. There seems to be somewhat better agreement in the later portion (summer) of 1992 than during the earlier time period shown in Plates 8 and 9, at least at 22 and 46 hPa. There may be some improvement based upon newer retrievals (discussed below), which take into account the effect of HNO<sub>3</sub> on ozone and include updated O<sub>2</sub> spectroscopic parameters, but full confirmation of this will have to await reprocessing of MLS data. We also note that least squares fits to the ozonesonde profiles (one of the smoothing methods mentioned earlier) produce much better agreement with the MLS data (notably at 46 hPa, where the 20% bias shown here essentially disappears); however, the smoothing method using the averaging kernels (ideally the method of choice) does not lead to such an improvement, so we cannot make a robust statement about this without more detailed analyses. As can be seen in Figures 24 and 25, the standard deviations of the differences are again about twice the estimated rms precision, in many instances, with implications as discussed above. Rms differences are overall not very different than those shown for the Boulder and Hilo sites.

**Gardermoen site.** Plate 10 and Figure 26 are similar in format to the above comparisons, but they apply to the Norwegian site of Gardermoen. The sonde data we obtained here cover about a year, but for 1993 (and one sounding in early 1994) as opposed to the earlier portion of the UARS mission. Also, although the total number of ozonesonde profiles is not much different than other comparisons above, these data are weighted fairly heavily toward the winter period. Although atmospheric variability and dynamics might be expected to play a bigger role for the comparisons at this site, especially in or near the winter polar vortex, the rms differences of Figure 26 are similar to those obtained from the tropical and midlatitude ozonesonde comparisons shown above. In fact, a significant part of these differences are systematic in nature, as can be seen by the  $\sim 0.3$  ppmv bias between MLS ozone and the sonde data (MLS values being higher); this amounts to a few to 10% overestimate by MLS, except at 100 hPa where the percentage difference is about 40%. Trends are generally well reproduced by both data sets, and the standard deviations of the differences are close to those shown above for other sites.

**McMurdo site.** The last ozonesonde data set we present is for McMurdo, Antarctica, where the period of most interest is during the occurrence of the ozone hole. The time span covered by the combined MLS and sonde observations over McMurdo for 1992 is from late August to mid-September, along with one coincidence in late October (see the time series comparison in Plate 11). Rather good agreement is observed in the ozone values and variations at 10 and 22 hPa; in particular, the large increase in ozone abundances which has occurred by late October is tracked very closely by both MLS and sonde data (see also at 46 hPa). At 46 hPa the September decline in ozone is seen in both data sets, although MLS values tend to be systematically lower than the sonde data. A consistent overestimate of the (sonde) ozone values by MLS data at 100 hPa is observed, even if one can argue that the large estimated errors in MLS ozone at this level can explain the differences. This overestimate is even larger than in the high northern latitude (Gardermoen) case, and a factor of 2 difference exists here in the average profiles (for September 1992), with 1.5 ppmv for MLS versus 0.7 ppmv for the sonde, as seen in Figure 27. This is caused in part by the occurrence of unrealistic ozone “bulges” at 100 hPa in some of the MLS profiles, where 100 hPa ozone values are larger than the 46 hPa values. Such features are not observed in the ozonesonde data and the MLS retrievals need a systematic improvement in this respect at 100 hPa, regardless of the nonnegligible noise level of individual retrievals at this height. We are investigating this issue to assess whether this might be related to poor knowledge of “contaminant” species (such as H<sub>2</sub>O, N<sub>2</sub>O, or HNO<sub>3</sub>) in this region at this time. However, it is worth noting that the standard deviations of the differences are smaller for McMurdo than for other sites considered (especially at 10 hPa), indicating good tracking between the two data sets, regardless of any biases.



**Figure 23.** Statistics of comparisons between MLS ozone profiles and coincident Hilo ozonesonde data presented in Plate 7; format is same as for Figure 22.

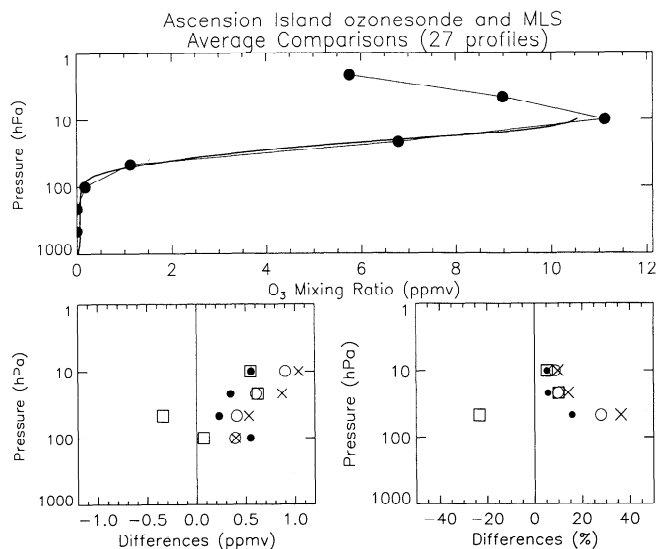
**Summary.** Figure 28 summarizes data from the six ozonesonde sites mentioned above, as compared to MLS ozone, in terms of average values at 100, 46, 22, and 10 hPa, along with average and rms differences in parts per million by volume and percent. Even though the time periods of observation are not identical, this indicates how latitude variations from averaged ozonesonde data are reproduced by MLS coincident profiles. Even at 100 hPa the average trends with latitude look encouraging. Sensitivity tests with latitude-independent a priori ozone indicate that the retrieved latitudinal variation is to a large degree unaffected by the choice of a priori, even at this pressure level (the variation observed by MLS is not, to first order, “caused” by the a priori, because of poorer measurement sensitivity). In some instances (especially at high latitudes) an MLS overestimate of ozone at 100 hPa exists, although we note that only half of the data sets used in the comparisons here show this as a significant problem. The general development of the ozone hole and the spring-time recovery is well followed by MLS data, in accord with average column ozone comparisons versus TOMS in the polar region [see Froidevaux *et al.*, 1994]. However, given the biases as well as the random errors, MLS ozone (Version 3 data) at 100 hPa cannot be considered reliable for detailed scientific analyses. At 46 hPa, there is a tendency for MLS data to lie below the ozonesonde measurements by a few tenths of a ppmv (except at Gardermoen, where the bias is reversed in sign). Some of the above differences may be related to closure problems in the simulations (see discussion of section 4), and some reduction in this bias is obtained when the sonde profiles are smoothed (or fitted) to a coarser (MLS-like) resolution; we note that this bias is also observed in comparisons with the 183-GHz MLS ozone data. Further analyses of this issue will be conducted after the next software upgrade. At 10 and 22 hPa, mean differences are systematically close to 5%, with MLS ozone

values higher than the sonde data; rms differences generally vary between 5 and 15%. Temporal variations observed in the sonde data (as displayed in previous plots) are generally well tracked by the MLS 205-GHz ozone retrievals, from 46 to 10 hPa.

### Comparisons With Ozone Data From Balloon Flights

We now present a summary of comparisons between MLS ozone data and midlatitude measurements obtained from large balloon flights between fall 1991 and spring 1994. The two data sets discussed here are the UV photometer (in situ) results (eight flights total) and the Submillimeter Limb Sounder (SLS) data, from remote sensing similar to the MLS technique. These two data sets were chosen primarily because they contain a significant number of profiles, even though it is clear that the frequency of these flights cannot match that of ozonesonde launches. The balloon flights were made either from Daggett, California (34.3°N latitude, 256.4°E longitude) or from Fort Sumner, New Mexico (34.9°N latitude, 243.2°E longitude), and we present average results for statistical reasons (and for brevity). Time series plots are not appropriate in this case, given the relatively poor temporal coverage of balloon flights. However, equinox conditions at midlatitudes have the advantage of providing a relatively static stratosphere, so that differences due to atmospheric variability can be minimized.

**UV photometer data.** The UV photometer is generally considered among the most accurate for ozone profile measurements [Hilsenrath *et al.*, 1986]. We have combined eight profiles from a UV in situ instrument launched aboard large balloons (which can reach somewhat higher altitudes than ozonesondes). Individual MLS and UV photometer ozone values (six of which are for profiles measured within ~300 km of each other, and all of which are within 900 km) are not shown here but compare quite well, i.e., essentially always within the estimated combined rms accuracies, of the order of 7% at best. A small bias emerges, however, between the two data sets, as seen from the average comparison profiles of Figure 29, and the bias accounts for a significant part of the rms differences between 22 and 5 hPa. The MLS ozone values are, as in the comparisons with ozonesondes, slightly higher than the UV data (by about 5%), near the ozone peak, from 5 to 22 hPa. Agreement at 46 and 100 hPa is better than 0.1 ppmv, but even such a small overestimate by MLS (versus the in situ data) can amount to ~20% at 100 hPa, where the mixing ratios are small (less than 0.5 ppmv). Rms differences for these comparisons are about 0.5 ppmv at all heights, which amounts to 5–20% between 4.6 and 46 hPa. For the estimated precision of the UV photometer, we have used 2% here, which would correspond better to the observed rms variability (at balloon float altitude for example) than the 5% canonical number used above for ozonesondes. The standard deviation of the differences in Figure 29 are reasonably consistent with (but gener-



**Figure 24.** Statistics of comparisons between MLS ozone profiles and coincident Ascension Island ozonesonde data presented in Plate 8; format is same as for Figure 22.

ally somewhat higher than) the estimated precision of the combined data sets.

**SLS data.** Ozone is measured by the SLS experiment [Stachnik *et al.*, 1992] from emission at 625 GHz, as the FOV scans through the atmosphere from the balloon at float altitude ( $\sim 38$  km); some information is also retrieved about the ozone abundance above this altitude, albeit with poorer accuracy. The SLS ozone profile averaged over the 5 midlatitude flights (all near equinox) is displayed in Figure 30, along with the corresponding average MLS profile and the sets of difference values. The differences are very small throughout the stratosphere, i.e., a few percent systematic difference (not really significant, given the relatively small number of coincident profiles), with the MLS values generally on the high side. We expect this small difference to be reduced when the newer MLS software, with updated O<sub>2</sub> spectroscopy, is used, since a few % reduction in ozone (at least above 10 hPa) is then likely (see section 8). The standard deviations of the differences between MLS and SLS are as small as any others presented above and are consistent with the combined error estimates shown; however, these estimates include values which represent accuracy (one sigma) rather than precision for the SLS data and the actual precision for the SLS profiles (which represent averages of many single profiles) is undoubtedly lower than the 5 % assumption made here. The main point, however, is that the average MLS and SLS profiles presented in Figure 30 are remarkably consistent.

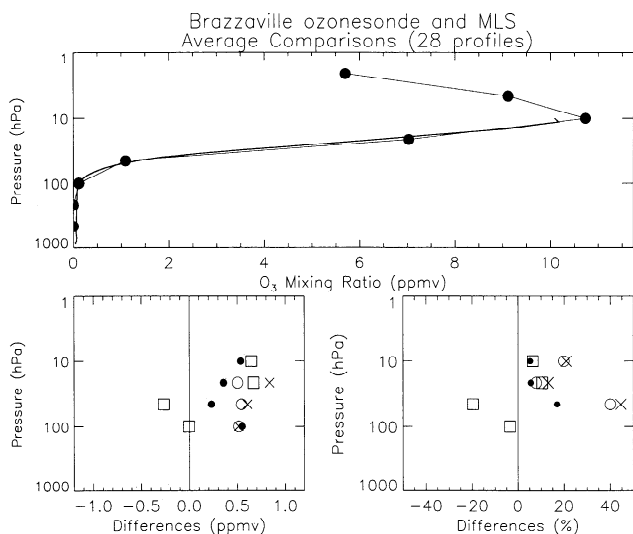
### Comparisons With Lidar Data

Summary comparisons between UARS data and lidar measurements of ozone are presented by Grose and Gille [1996]; Redaelli *et al.* [1994] have also discussed sample comparisons between MLS data and lidar data

from l'Aquila, Italy. We focus here on comparisons with the Table Mountain Facility lidar, which has acquired a large continuous ozone database since 1988 [see McDermid, 1993].

**Table Mountain Facility (TMF).** The TMF lidar data used here span the September 1991 to November 1994 time period. These data have been recently reviewed to screen obvious aerosol contamination and reprocessed, with changes in temperature affecting ozone mixing ratios (via the number densities). A temperature tie-on for the top of the profiles (near 80 km) is now used rather than a pressure tie-on and density normalization near 30 km (as used previously). The effect of this change is to reduce the sensitivity of the algorithms to aerosol contamination, for the upper part of the temperature profiles; this also helps to identify regions in the bottom part of the profile where aerosol contamination occurs. Furthermore, NMC data are now used to convert from altitude to pressure, whereas a model atmosphere [Keating *et al.*, 1987] was used before. Finally, a minor change in starting altitude for the background level estimation in one of the receiver channels has resulted in slightly lower ozone concentrations at the top of some lidar profiles. Overall, the changes in processing have led to a decrease of about 7% in the average lidar-inferred ozone at 1 hPa, with negligible effects (of the order of 1%) elsewhere. The decrease near the top of the lidar profiles should reduce the small systematic differences mentioned by Tsou *et al.* [1995] between TMF lidar data and ground-based microwave (and SAGE II) data.

Time series comparisons for about 3 years of MLS and TMF lidar data are displayed in Plate 12, and average profile comparisons are shown in Figure 31. Similar cycles (annual primarily) are observed in both data sets, with a transition from the midstratosphere (with peak values in late spring to early summer) to the upper stratosphere (where anticorrelation with temperature variations is expected). As we see from these two figures, the 10-hPa comparisons give results which are in better agreement (on average) than the other data sets shown above; namely, there is excellent agreement between the TMF lidar data and MLS ozone at this level, whereas a small but systematic 5% offset was evident in the other data set comparisons. If the ozonesonde data and UV results are considered as "truth," this would imply that both the TMF lidar and the MLS values are biased high (by about 5%) near 10 hPa. Plate 12 shows excellent tracking of the annual cycle at 10 hPa for MLS and lidar values, and Figure 31 gives rms differences close to 5% at this level (and at 4.6 hPa). Average differences between MLS and these reprocessed TMF lidar data are less than 5% over all heights; we do not show the statistics of differences at heights below 10 hPa because of the small number of lidar profiles (less than 10% of the total number of profiles) that exist down to the 22-hPa level, but the average agreement is good there as well. The standard deviations of the differences between MLS and lidar profiles increase with altitude, reaching 20% at 1 hPa; this could be in part



**Figure 25.** Statistics of comparisons between MLS ozone profiles and coincident Brazzaville ozonesonde data presented in Plate 9; format is same as for Figure 22.

because of larger atmospheric variability at the uppermost levels and also because of the reduced sensitivity of both instruments in that region.

#### Other data sets

The purpose of this section is to mention other ozone data sets for which we know some comparisons with MLS data exist; this can help place the above discussions in a broader context. First, a large number of profile comparisons between MLS ozone (from the 205-GHz band) and SAGE II ozone data have been performed and presented by *Cunnold et al.* [this issue (a)]. The general conclusion of that work is that MLS (Version 3) ozone values are about 5% larger than the SAGE II data, for the stratospheric values compared (down to about 30 hPa); this result is (to first order) not latitude or height dependent. This would tend to agree with a good fraction (but not all) of the comparisons shown in this paper for 10 and 22 hPa. However, the TMF lidar and MLS ozone comparisons (pressures of 1 to 10 hPa) do not show such a bias. This could be because the TMF lidar data also have a slight positive bias (with respect to “truth”); indeed, there are indications that those data are on the high side of other lidar and ground-based microwave ozone data [see *Grose and Gille, 1996*], but it is not clear that a sufficiently extensive study has been performed. Based on some of the analyses discussed by *Grose and Gille* [1996] and other comparisons (J. Gleason, private communication, 1994), MLS ozone zonal mean values are generally larger than the Solar Backscatter Ultra Violet (SBUV/2) mean data, by about 10 to 15%, with the amplitude of temporal variations larger in the MLS data set than in the SBUV/2 data (possibly in relation to the different vertical resolutions); an understanding of these differences will require further study. Another set of

ozone profiles of interest is the data set from the Atmospheric Trace Molecule Spectroscopy (ATMOS) experiment aboard the space shuttle (ATLAS missions); very encouraging comparisons are emerging from such studies (M. Abrams, private communication, 1994). Further comparisons of UARS ozone data sets can be found in the work of *Cunnold et al.* [this issue (b)]. Also, validation work of interest would involve the comparison of mapped products at a given pressure. General features certainly look similar among various instrument results (UARS and SBUV/2 global data), but there are some differences [e.g., *Grose and Gille, 1996*] which still need to be fully understood.

### 7. Precision and Accuracy of Version 3 Data

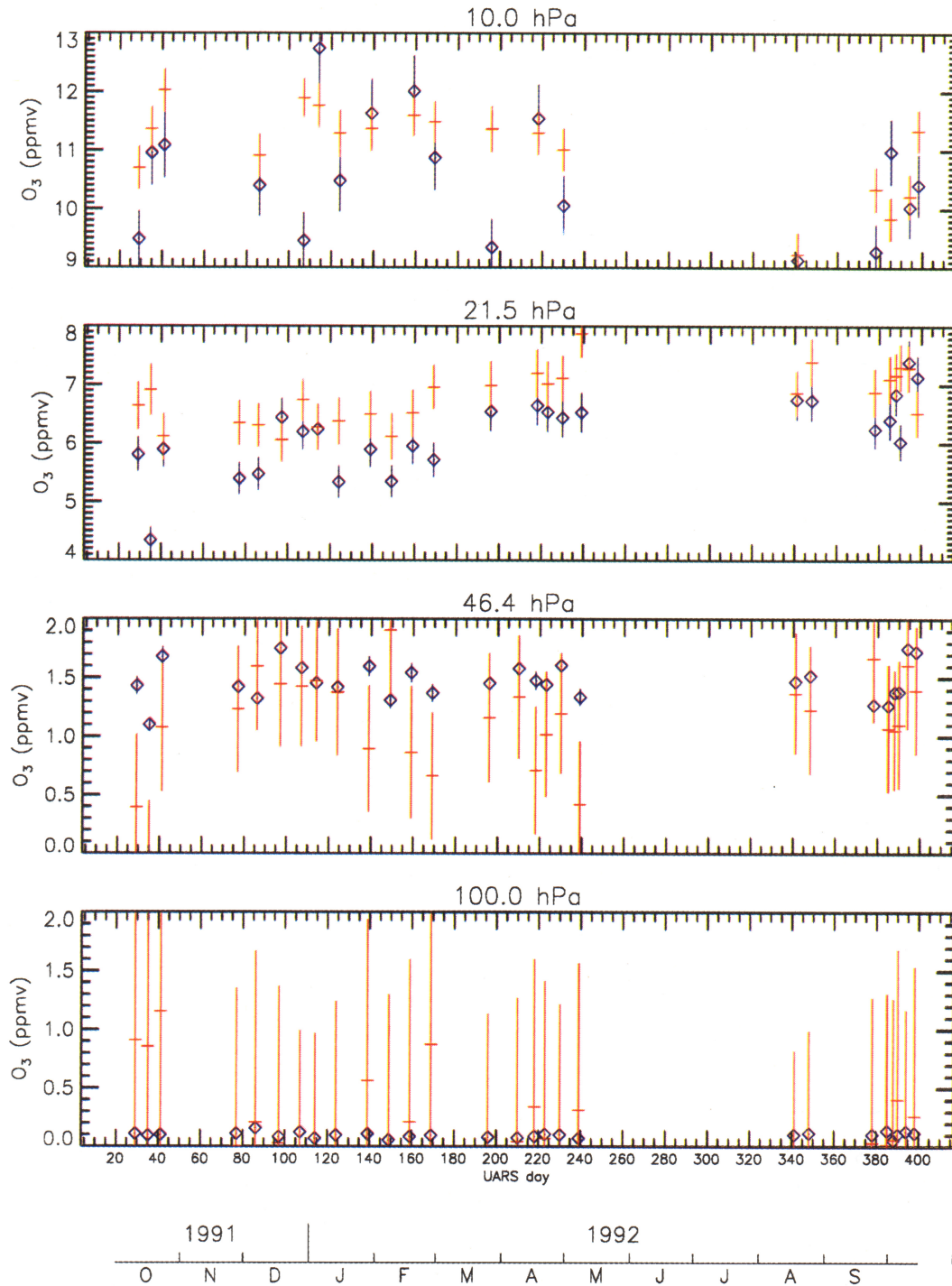
The evidence presented in this paper and the references to other comparisons mentioned here indicate that the MLS ozone data can be most reliably used in the 22- to 0.5-hPa region. Comparisons with some data sets which can be considered accurate to about 5% (i.e., UV photometer, ozonesonde, and SAGE II data) give 5 to 10% (or better) agreement. MLS data in this region tend to be about 5% larger than most of the correlative values. We will see in section 8 that this bias is likely to be reduced with a future MLS software version.

Tables 2a and 2b summarize our best estimates of precision (single profile) and accuracy for MLS Version 3 ozone data. We have derived estimated accuracy values as a function of height by using the root sum square of the estimated systematic uncertainties and the a priori contributions given in section 5. Even though the a priori error contribution, or smoothing error [see *Marks and Rodgers, 1993*] is treated as a random component in a theoretical sense [*Rodgers, 1990*], we include it here as part of the accuracy figures, since averaging many MLS ozone profiles in an altitude region of poor measurement sensitivity (e.g., at or above 0.1 hPa for 205-GHz ozone data) would, in the extreme case, give a climatological value with error quite possibly larger than the systematic uncertainty. By using this approach, one is kept aware of the fact that there are regions where the measurements should not be considered reliable. For ozone data from the 205-GHz band, rounded-off values are close to 0.3 ppmv from 22 to 0.5 hPa and slightly under 0.6 ppmv at 46 hPa; the estimated accuracy at 100 hPa for the current retrievals is best expressed as being of the order of 50% or larger, given the wide relative range of possible ozone mixing ratios (from tropics to poles) at this altitude. We choose to round the estimates off (generally on the high side) because these numbers are estimates with probably one only significant digit (past the decimal point). If we compare these values to typical residual errors, we find good agreement and see no reason to change the estimates based on the radiance fits. Based on the comparisons given in section 6 and the overall biases noted there, we also see little reason to change our estimates of accuracy (except at 46 hPa, see below). Indeed, these are to be used as “one sigma”

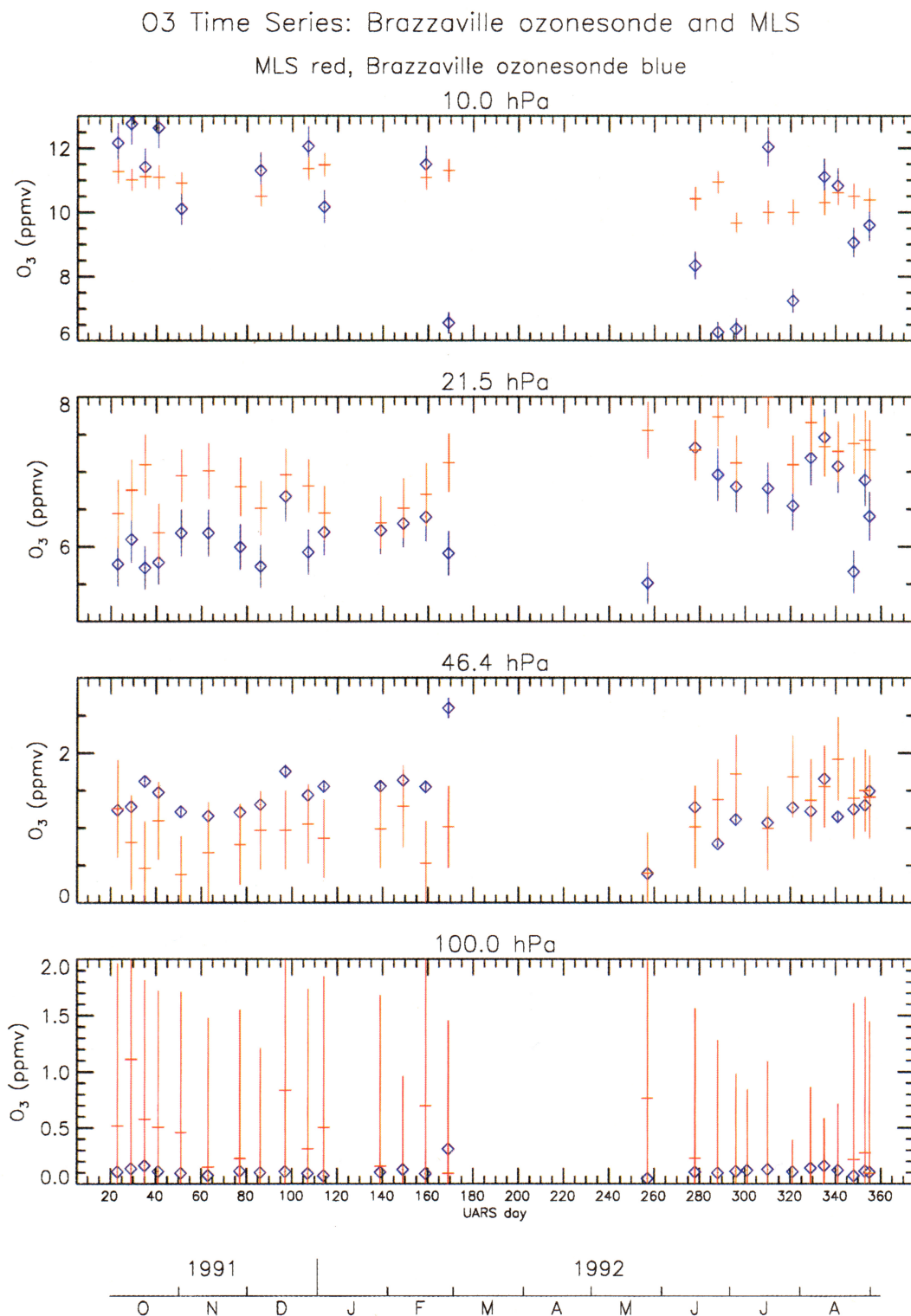


O<sub>3</sub> Time Series: Ascension Island ozonesonde and MLS

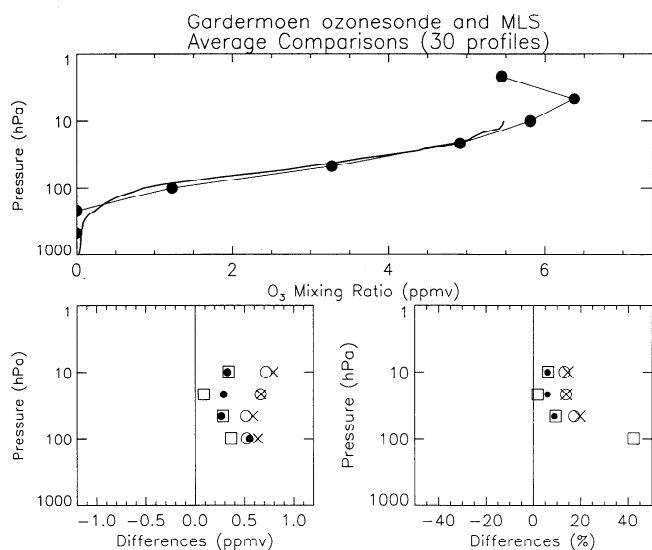
MLS red, Ascension Island ozonesonde blue



**Plate 8.** Time series comparison between MLS ozone mixing ratios (ppmv) at 100, 46, 22, and 10 hPa (bottom panel to top panel) and Ascension Island ozonesonde data during 1991–1992 (27 coincident profiles total); format is same as for Plate 6.



**Plate 9.** Time series comparison between MLS ozone mixing ratios (ppmv) at 100, 46, 22, and 10 hPa (bottom panel to top panel) and Brazzaville ozonesonde data during 1991–1992 (28 coincident profiles total); format is same as for Plate 6.



**Figure 26.** Statistics of comparisons between MLS ozone profiles and coincident Gardermoen ozonesonde data presented in Plate 10; format is same as for Figure 22.

estimates, and the biases (and certainly the rms differences) between MLS and other data sets provide at best an upper limit to the MLS accuracy (since the other data sets do not have perfect knowledge and true atmospheric variability affects the rms differences). In fact, we believe that the estimated accuracy is too large at 46 hPa, given the comparisons of section 5 (where the absolute differences at 46 hPa are not typically worse than at other pressures). Therefore in the tabulated recommendations for 205-GHz ozone accuracy (see Table 2a) we have used a value of 0.4 ppmv (not 0.6 ppmv) at 46 hPa (or 20%) as a guide. Indeed, this table is to be used as a guide, and the reader can look at the latitude dependence of the comparisons in section 6 for further information on likely accuracy. We note, furthermore, that while Tables 2a and 2b are not inconsistent with the quality of simulation results discussed in section 4, we cannot convey all the information from that section or the comparison results in one table. In terms of precision, comparisons with other data sets and repeatability estimates for the MLS data indicate that the measurement noise contribution estimates of section 5 are reasonable; we believe that atmospheric variability and noncollocation of measurements accounts for the additional variability in the differences between MLS and other data sets.

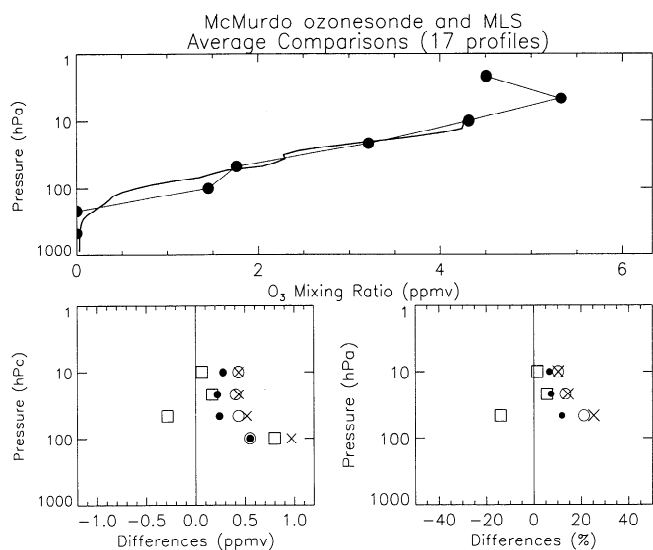
For 183-GHz ozone data the estimated values from a priori and systematic error contributions given in section 5 provide the basis for the tabulated accuracies in Table 2b. Given the agreement (within the combined precision of the two ozone data sets) generally found between the 205- and 183-GHz ozone data, the actual accuracy of the 183-GHz data is probably better than given in the table. However, the adjustment to the FOV-pointing alignment for the 183-GHz radiometer contains a semiempirical component, and there is

no doubt that, without other sources of information, the 183-GHz data are intrinsically less accurate than the 205-GHz data. Also, the existence of larger radiance residuals supports this assertion. Typical residual errors would appear to be slightly lower than the tabulated values but not overwhelmingly so (see discussion at end of section 5).

With the information contained in this paper on possible small biases in the current MLS ozone values, keeping in mind again that “truth” is not rigorously known at much better than the 5% level of uncertainty, the user can hopefully decide the level of significance to attach to results obtained with this data set. It is not easy to assign a possible systematic error at the 5% level to one particular cause, and a combination of factors could play a role, given the error sources discussed in section 5. The most likely sources of this kind of potential 5% bias (based on the comparisons in section 6), particularly since it appears to occur in the upper stratosphere where contaminant species play a negligible role, would arise from small errors in tangent pressure registration (an error in the O<sub>2</sub> 63-GHz line width and/or an error in FOV direction for the 205-GHz radiometer) or in the 205-GHz ozone line width itself. We also saw that the likely sources of systematic error for the 183-GHz ozone retrievals include the above factors (with FOV direction errors accounting for an even larger contribution than in the 205-GHz radiometer case), along with a significant uncertainty in the knowledge of sideband ratios. It is possible that the reason for an apparent disagreement between the FOV misalignment estimate obtained from Moon scan analyses and the estimate obtained from a comparison between 205- and 183-GHz ozone data sets is because of a compensating error in the sideband ratio values for the 183-GHz radiometer. Such issues may be difficult to resolve completely, but continued investigations are planned.

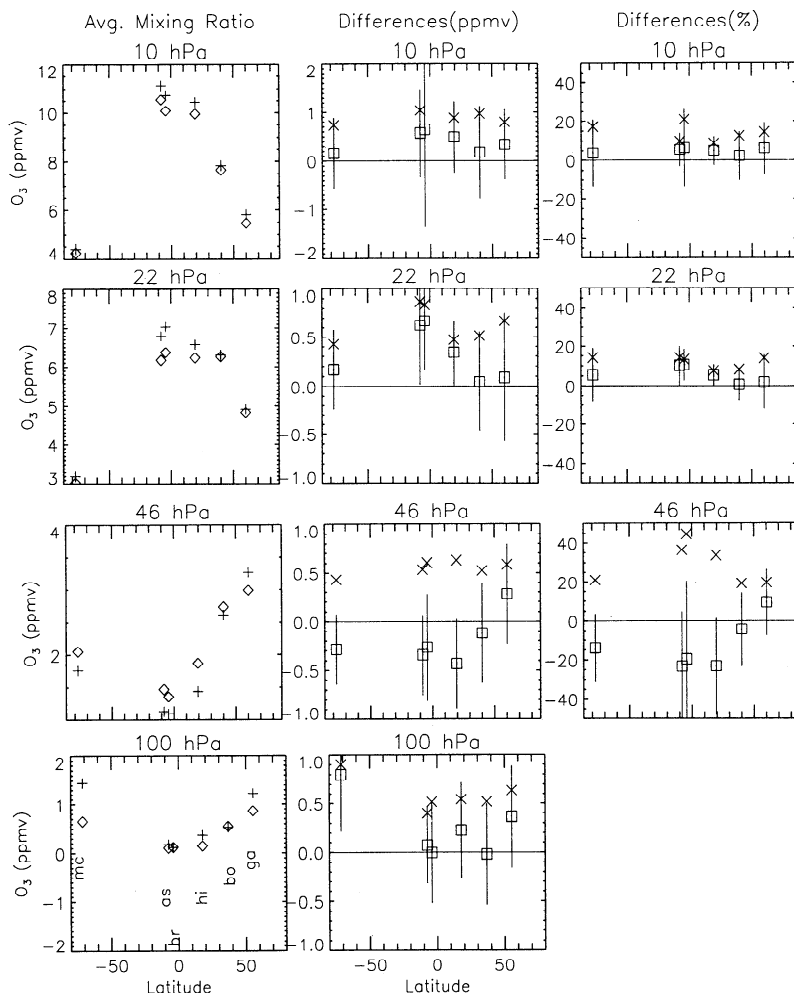
## 8. Plans for Further Work

A test version of software with recent updates is briefly discussed here in terms of expected changes in the future. One of the main changes involves retrievals of HNO<sub>3</sub> using the band 4 radiances (also used for retrievals of the 205-GHz ozone data); updated spectroscopic data for this molecule have also been obtained (E. Cohen, private communication, 1994). In addition to providing HNO<sub>3</sub> data, this can provide some improvement in the ozone radiance residuals and may give somewhat improved ozone values. The other main change is the inclusion of updated spectroscopic data for band 1 (63-GHz O<sub>2</sub> line width data), based on Liebe *et al.* [1992], which amount to a 6% narrower line width. Other minor changes deal with better modeling (in the forward model) of the sideband ratio gradients within channels, a radiance interpolation scheme for the use of radiance values at a tangent point pressure of 100 hPa (for slightly better information content in that region) and a smoother set of a priori (“climatological”) val-

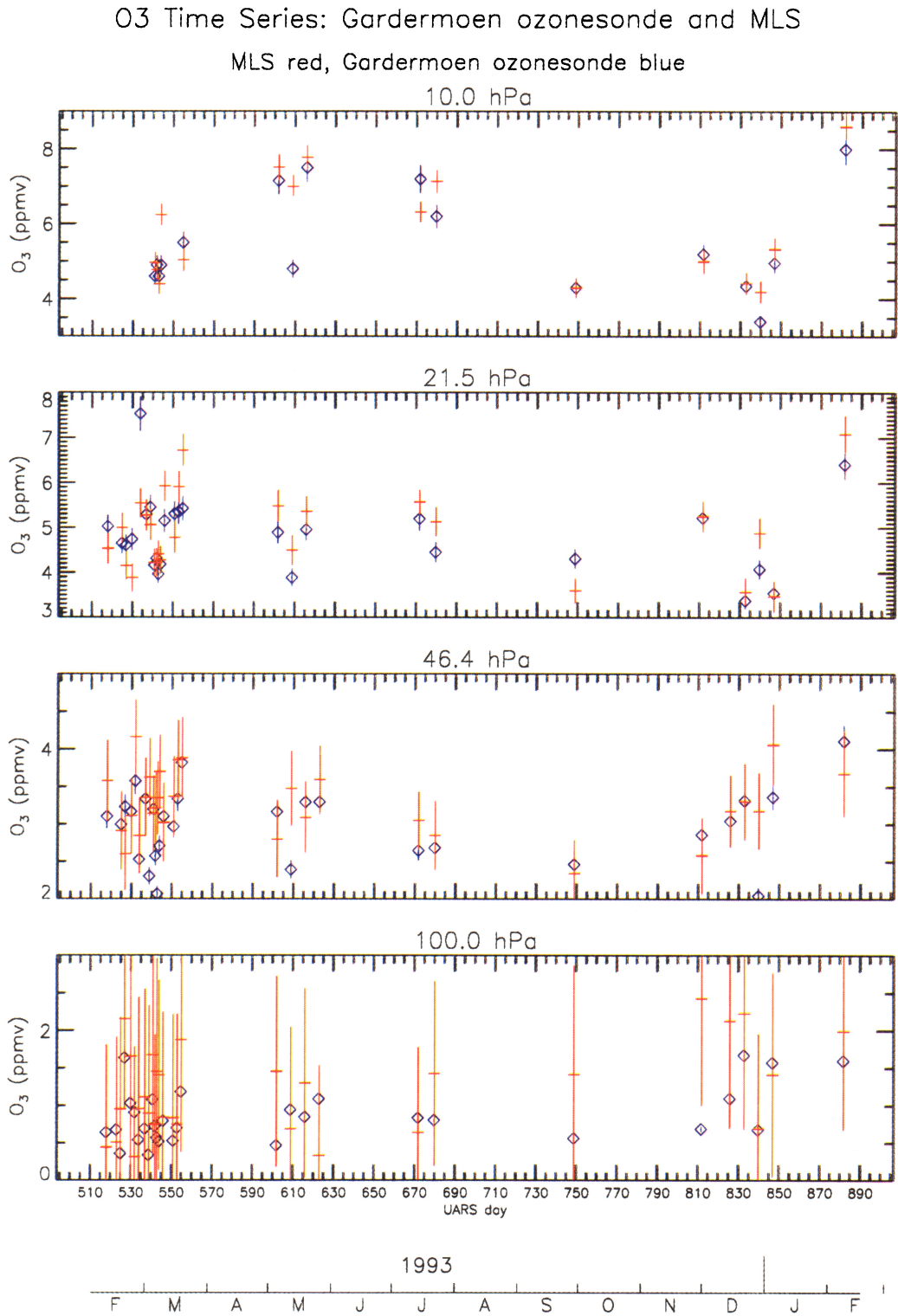


ues for the mixing ratios, to fill in some gaps. Figure 32 gives a summary of ozone results from this updated software (for a 1-day run). We observe a small decrease in ozone above 10 hPa, increasing from 0% (at 10 hPa) to a maximum of 6% in the upper stratosphere, with very little latitude dependence; this is a result of the lower (by about 200 m) tangent altitudes retrieved using the newer O<sub>2</sub> spectroscopy [see *Fishbein et al.*, this issue]. Increases in ozone are observed in the lower stratosphere, reaching 20% at 46 hPa, with some latitude dependence in the amount of increase; this is largely caused by the inclusion of HNO<sub>3</sub> in the

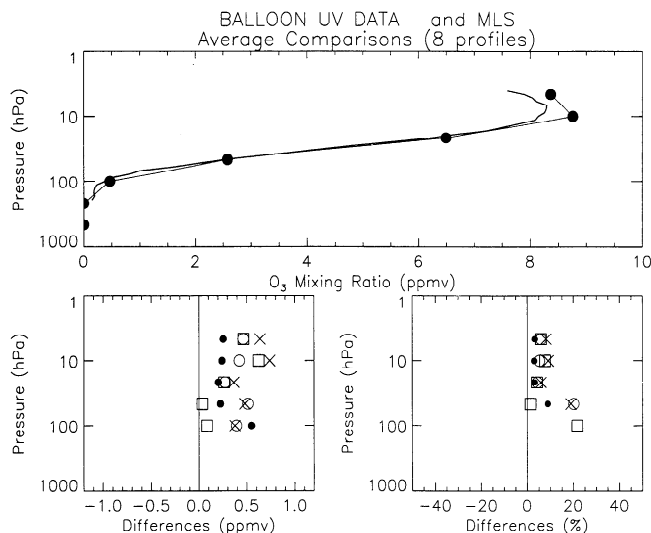
**Figure 27.** Statistics of comparisons between MLS ozone profiles and coincident McMurdo ozonesonde data presented in Plate 11; format is same as for Figure 22.



**Figure 28.** Latitude dependence of the ozone comparisons between MLS 205-GHz band data and ozonesonde data, based on the average data presented in Figures 22, 23, 24, 25, 26, and 27. Each panel in a given column corresponds to a different pressure level (as indicated above each panel). In the left column, average MLS mixing ratios (plus symbols) are compared to the average sonde data (open diamonds) for each of the six sonde locations. Each site is identified by lower case letters (first two letters of site name) in the bottom left panel. The middle column gives average (open squares) and rms (crosses) differences (MLS minus sonde), in parts per million, while the right-hand column shows these differences in percent. We have omitted the 100-hPa panel on the bottom right, since ozone values get too small to be satisfactorily compared in percent.



**Plate 10.** Time series comparison between MLS ozone mixing ratios (ppmv) at 100, 46, 22, and 10 hPa (bottom panel to top panel) and Gardermoen ozonesonde data during 1993–1994 (30 coincident profiles total); format is same as for Plate 6.



**Figure 29.** Statistics of comparisons between MLS ozone profiles and coincident UV photometer measurements from balloon. Format is same as Figure 22. Shown are the average profiles and differences, for MLS and UV photometer data obtained near 33°N. Balloon flights occurred on October 1, 1991; May 29, 1992; September 29, 1992; May 31, 1993; September 25, 1993; and May 22, 1994, from near Fort Sumner, New Mexico, and on February 20, 1992, and April 3, 1993, from Daggett, California. MLS data were generally obtained within 12 hours of the flight, except for the May 22, 1994, flight, when UARS was not operational; an MLS profile from May 24 was used in this case, which is not unreasonable for this time period of low variability.

retrievals. For the 183-GHz ozone retrievals, the HNO<sub>3</sub> retrievals play no role, and the newer software predicts a decrease of the order of 5 to 10% in most regions, with only a small (1%) increase at 22 hPa. However, we observe a significant improvement in the radiance fits (values of  $\chi^2_{ma}$  drop from about 14 to 4, on average), with similar improvements in band 5 (H<sub>2</sub>O retrievals), with the newer software, which gives us some added confidence in the updated O<sub>2</sub> spectroscopy and resulting tangent pressures. The bottom panel of Figure 32 gives the percent difference between the 183- and 205-GHz ozone data for this newer software. Most of the differences are not significant (given the uncertainties), but the systematic difference at 46 hPa (of the order of 30%, with 183-GHz retrievals producing lower values) will require further investigation. The accuracy of ozone values at 100 hPa has not been improved by this newer software, and more work is needed to resolve the existence of artifacts noticed in that altitude region in particular (see section 4). Significant improvements in this region will require better modeling/knowledge of the lower stratospheric continuum and contaminant species, including better H<sub>2</sub>O retrievals, and a nonlinear retrieval scheme (for optimum use of all channels, especially at 183 GHz).

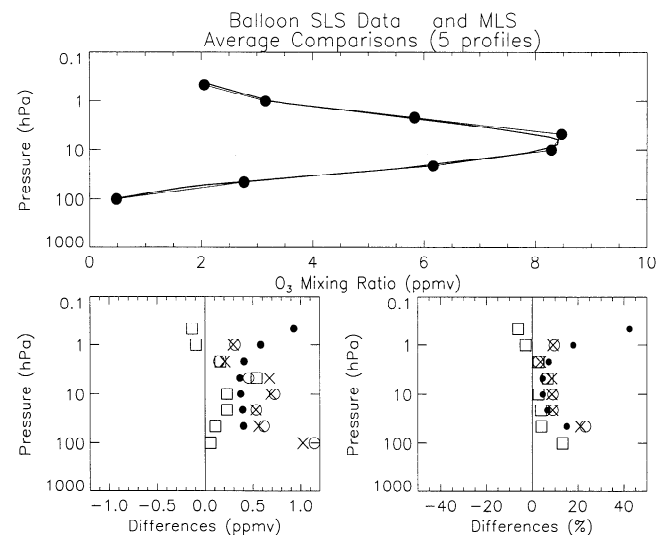
Finally, the vertical resolution of the retrieval grid can be improved, even though the precision at a given level would be degraded. Figure 33 shows the trade-off between vertical resolution and precision, for the

205-GHz ozone retrievals, assuming the current a priori errors (mentioned in section 3). An optimum retrieval grid spacing of about 3 km appears to exist, although it may be more desirable to retrieve on the actual UARS Level 3 grid points, which are only slightly closer in spacing. We intend to explore these options further for future upgrades to the software.

## 9. Conclusions

The MLS ozone data have been discussed from the point of view of their internal consistency (radiance closure), as well as in comparison to other reliable data sets. Precision and accuracy estimates for both the 205-GHz and 183-GHz data (MLS Version 3 files) have been given, and likely sources of error have been presented.

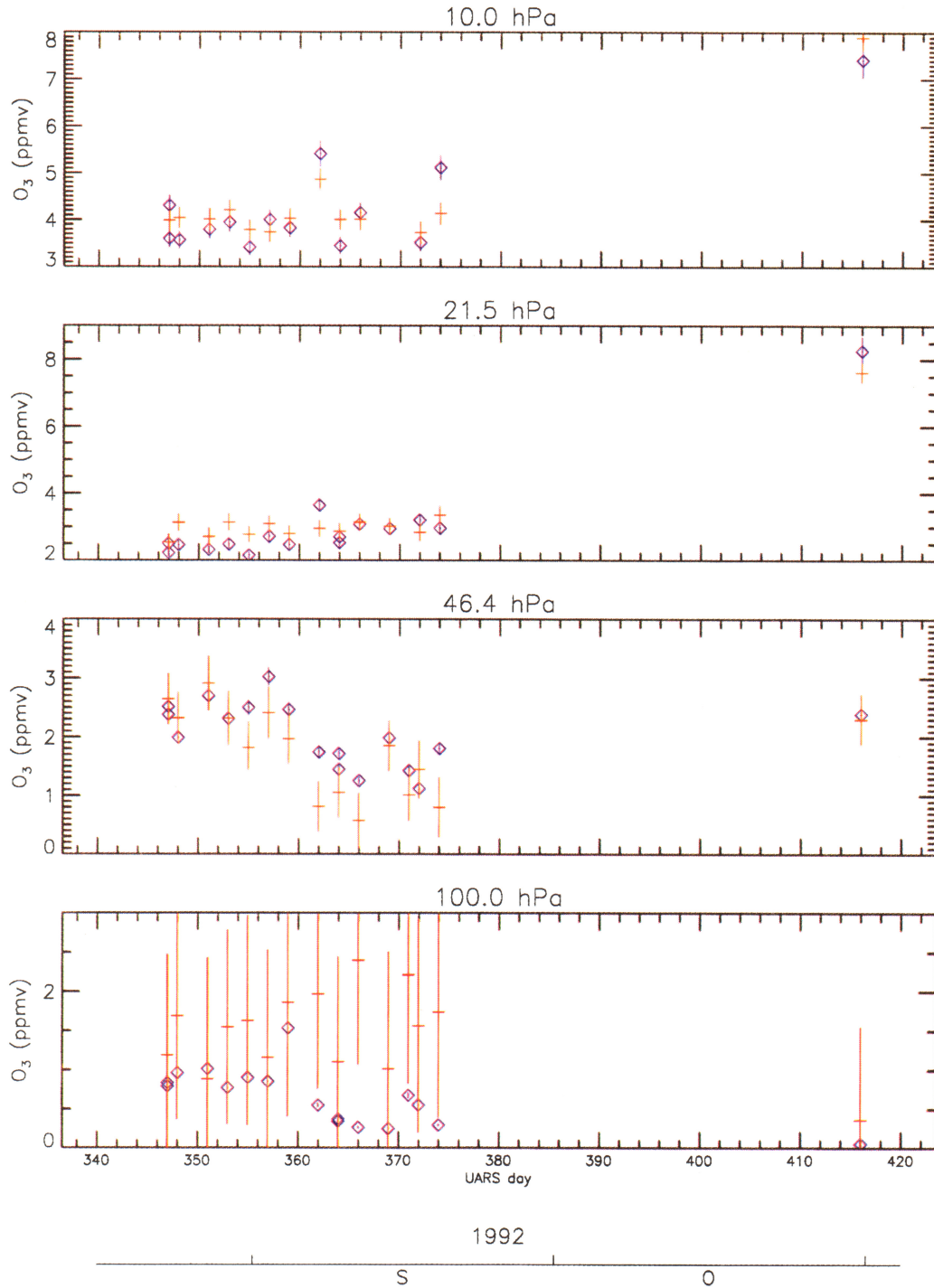
We find that the vertical range of usefulness for the Version 3 (205-GHz) data is 46 to 0.46 hPa, with 100-hPa retrievals not yet consistently reliable. MLS data in the uppermost stratosphere (data between 1 hPa and 0.46 hPa) have not been scrutinized as thoroughly as in the lower-altitude range, mostly because of the relative paucity and poorer quality of correlative data sets at the upper levels; see *Cunnold et al.* [this issue (a and b)] for more information on UARS ozone data validation at these heights. The rms precision is of the order of 0.2 ppmv throughout most of the stratosphere, with estimated (rms) accuracy of the order of 0.3 ppmv ( $\sim 3\%$  to more than 50% for 100 hPa). A large part of the radiance closure problems in the lower stratosphere will be remedied, it seems, by the inclusion of HNO<sub>3</sub> retrievals; better knowledge of other contaminant species (such as H<sub>2</sub>O and N<sub>2</sub>O) and tangent pressure will also help. Also, revised O<sub>2</sub> spectroscopic parameters should help reduce the slight (5% or so) MLS overestimate of ozone which may exist in the middle to



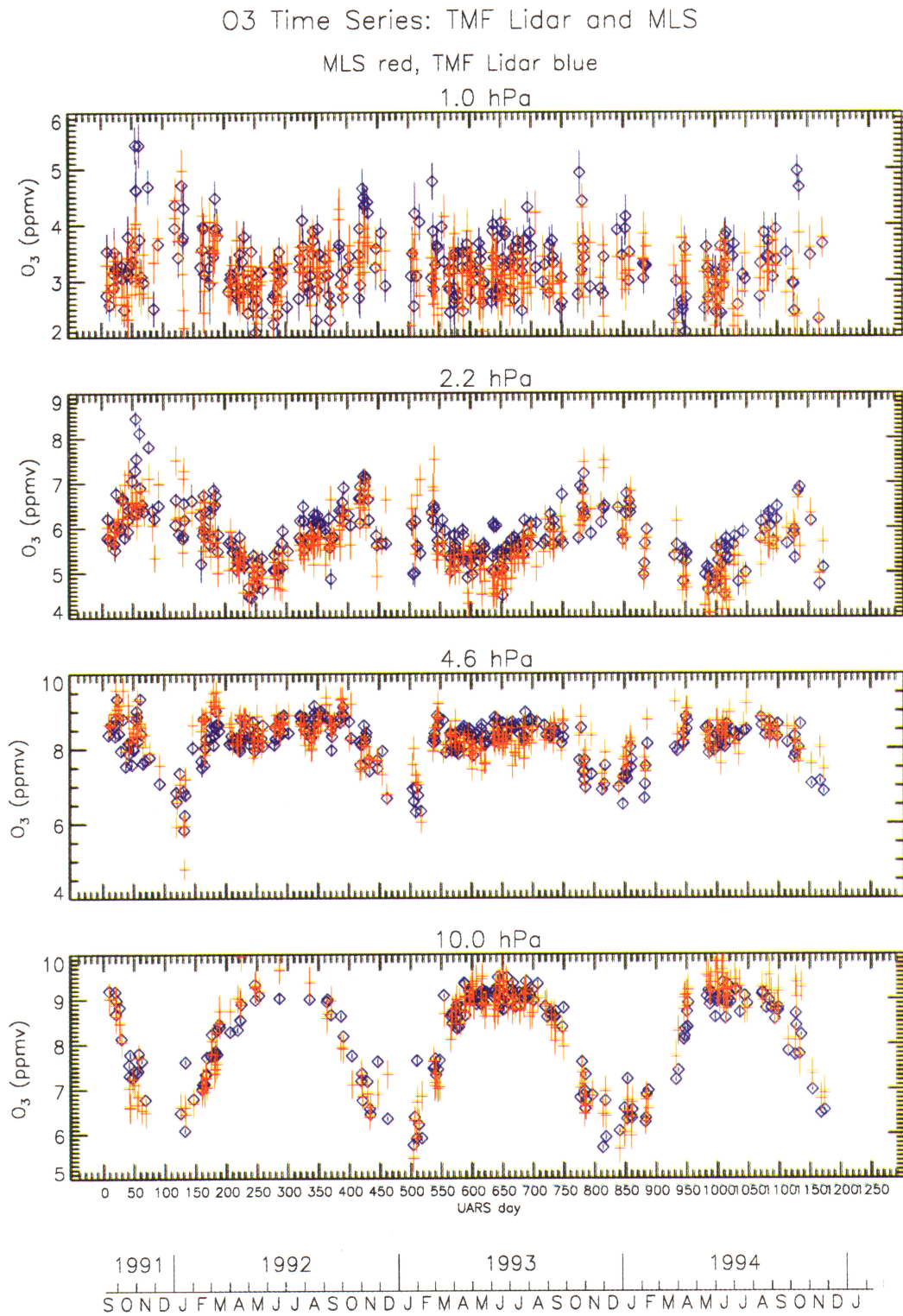
**Figure 30.** Average profiles (and difference quantities, as done in previous figures) for MLS and Submillimeter Limb Sounder (SLS) data from a total of five balloon flights from Daggett, California, and Fort Sumner, New Mexico. The dates are as in Figure 29, except for the May 1993 and 1994 flights, when the SLS did not participate.

O<sub>3</sub> Time Series: McMurdo ozonesonde and MLS

MLS red, McMurdo ozonesonde blue

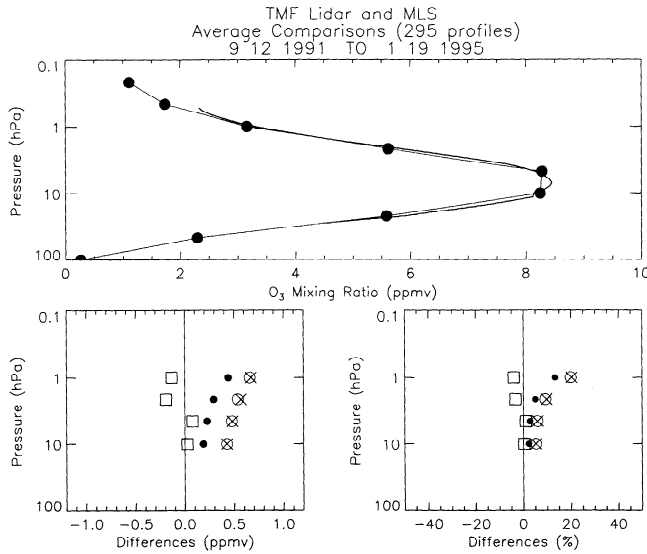


**Plate 11.** Time series comparison between MLS ozone mixing ratios (ppmv) at 100, 46, 22, and 10 hPa (bottom panel to top panel) and McMurdo ozonesonde data during August to October, 1992 (17 coincident profiles total); format is same as for Plate 6.



**Plate 12.** Time series comparison between MLS ozone mixing ratios (ppmv) at 10, 4.6, 2.2, and 1 hPa and Table Mountain Facility (TMF) lidar data during 1991–1994. Format is same as for Plate 6.





**Figure 31.** Statistics of comparisons between MLS ozone profiles and coincident lidar data presented in Plate 12. Format is same as in Figure 22. The differences in the bottom panels do not include levels below 10 hPa, because of the small number of lidar profiles extending down to the 22-hPa level.

upper stratosphere (through more accurate retrievals of tangent pressure). At the sub-5% level, it becomes difficult to rigorously demonstrate that one data set is the closest one to “truth.” Issues such as the differ-

ent vertical resolution of various instruments are worth considering. While there are indications that this effect plays a role in the tropical differences (of the order of 20 %) between MLS and ozonesonde data at 46 hPa, we cannot fully explain these differences at this point; this will be revisited after the next software upgrade.

For MLS Version 3 ozone values retrieved from the 183-GHz radiometer data, the stronger line can lead to more precise measurements in principle; however, radiance closure analyses and absolute mixing ratios after launch pointed to the existence of larger systematic effects in this data set, most likely as a result of poorer calibration knowledge. The optimum use of all channels in the future should improve the situation, especially in the middle to lower stratosphere, and the stronger line and relative lack of contaminant species are an advantage for this data set. The currently recommended vertical range of usefulness is 46 to 0.046 hPa for 183-GHz ozone results, but we recommend the 205-GHz data for the stratosphere and the 183-GHz data for the mesosphere (because of the larger signal to noise). Significant improvements in closure are known to occur when updated O<sub>2</sub> spectroscopy is used.

Future iterative retrievals will produce improved MLS data sets. Other engineering issues, like increasing the spectral bandwidth, will improve future lower stratospheric measurements planned for the Earth Observing System (EOS) MLS; note that the UARS MLS instrument was not originally designed for the lower stratosphere, when chlorine-catalyzed ozone depletion

**Table 2a.** Estimated Precision and Accuracy of MLS 205 GHz Ozone

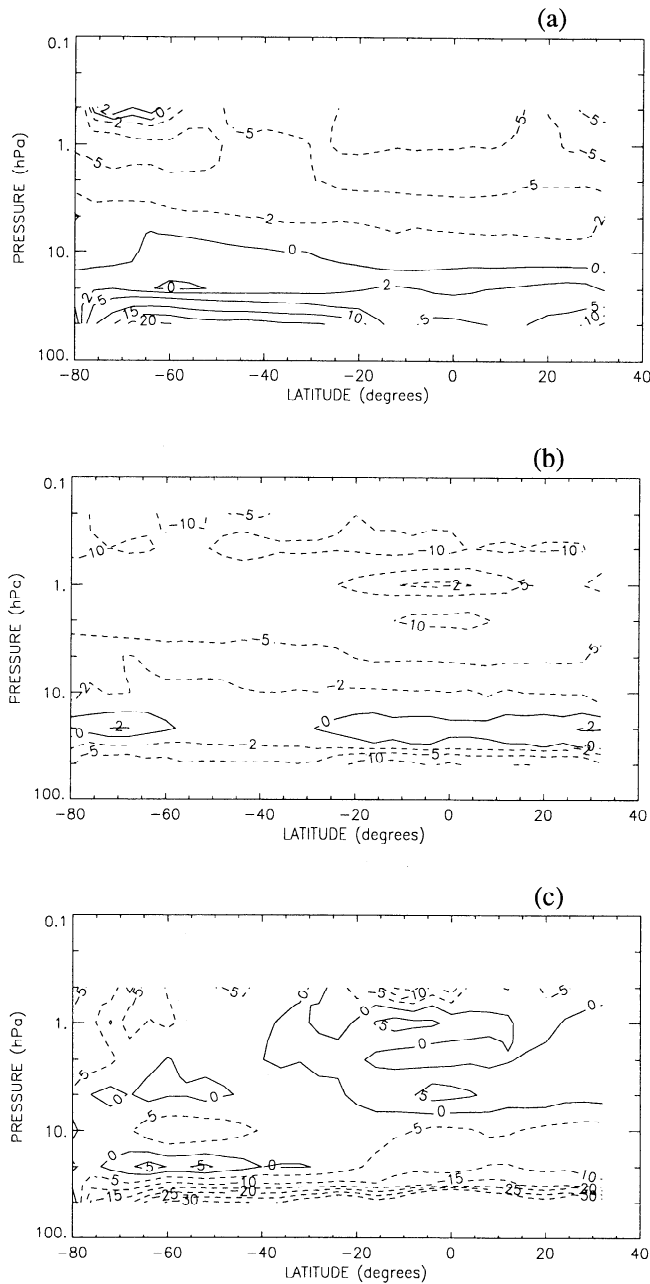
UARS Level	Pressure, hPa	Precision		Accuracy	
		ppmv	percent	ppmv	percent
20	0.46	0.37	20	0.3	15
18	1.0	0.31	10	0.3	10
16	2.2	0.23	4	0.3	5
14	4.6	0.20	2	0.3	5
12	10	0.18	2	0.3	5
10	22	0.16	3	0.4	5
8	46	0.22	11	0.4	20
6	100	0.55	≥50		≥50

Precision given here is for individual profiles.

**Table 2b.** Estimated Precision and Accuracy of MLS 183 GHz Ozone

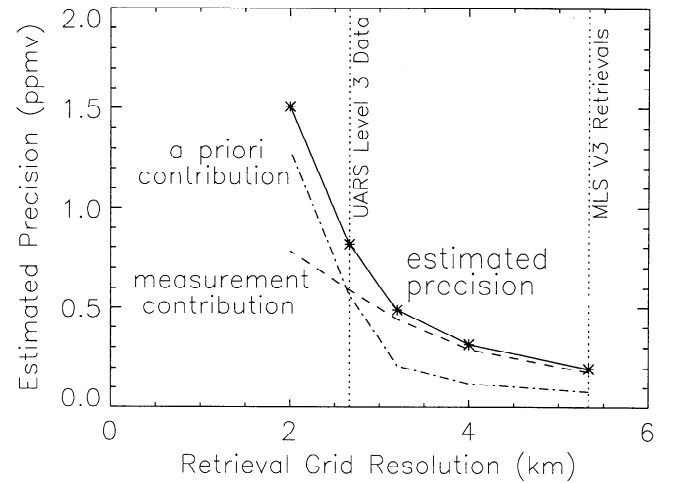
UARS Level	Pressure, hPa	Precision		Accuracy	
		ppmv	percent	ppmv	percent
26	0.05	0.30	55	0.5	≥50
24	0.10	0.26	30	0.3	35
22	0.22	0.17	17	0.2	20
20	0.46	0.10	6	0.2	10
18	1.0	0.10	3	0.4	15
16	2.2	0.10	2	0.8	15
14	4.6	0.10	1	0.9	10
12	10	0.13	2	0.9	10
10	22	0.20	3	0.8	15
8	46	0.10	6	0.8	45

Precision given here is for individual profiles.



**Figure 32.** Comparison of Version 3 MLS data with recently updated software (see text), for Aug. 29, 1992. (a) Zonal mean % differences (new minus old values) for 205-GHz ozone, (b) 183-GHz ozone, and (c) zonal mean % differences for ozone 183-GHz minus 205-GHz data in the updated software (to be compared to differences shown in Figure 15 for Version 3 MLS data).

was thought to be mainly an upper stratospheric issue. The information and caveats in this paper should allow for a more informed group of researchers to appreciate the quality of currently available MLS ozone data and to proceed in their analyses with more confidence (or more caution in some cases). We look forward to providing even better data sets from MLS in the future, with optimum use of this instrument's capabilities.



**Figure 33.** Trade-off between vertical resolution (of retrievals) and uncertainty in 205-GHz ozone at 46 hPa. Total uncertainty (ppmv), for a 3 ppmv a priori error, is plotted versus retrieval grid resolution (km).

### Appendix: Combination of a Priori and Measurement Information

Starting with measurements  $\mathbf{y}$  with error covariance  $\mathbf{E}$ , and an assumed linear relation (via weighting functions  $\mathbf{K}$ ) to state vector  $\mathbf{x}$  (or more accurately, a linear relation between departures of these quantities from true or a priori values), the well known weighted least squares solution for  $\mathbf{x}$  and its error covariance  $\mathbf{S}$  is

$$\hat{\mathbf{x}}_{LS} = (\mathbf{K}^T \mathbf{E}^{-1} \mathbf{K})^{-1} \mathbf{K}^T \mathbf{E}^{-1} \mathbf{y}, \quad (\text{A1})$$

$$\hat{\mathbf{S}}_{LS} = (\mathbf{K}^T \mathbf{E}^{-1} \mathbf{K})^{-1} \quad (\text{A2})$$

The above solution minimizes the sum of the squared residuals  $(\mathbf{y} - \mathbf{K}\mathbf{x})^T \mathbf{E}^{-1} (\mathbf{y} - \mathbf{K}\mathbf{x})$ . Also, given two estimates  $\mathbf{x}_1$  and  $\mathbf{x}_2$  of quantity  $\mathbf{x}$ , with error covariances  $\mathbf{S}_1$  and  $\mathbf{S}_2$ , the maximum likelihood (or optimum) estimate of  $\mathbf{x}$  and its error covariance  $\mathbf{S}$  can be written as:

$$\mathbf{x} = (\mathbf{S}_1^{-1} + \mathbf{S}_2^{-1})^{-1} (\mathbf{S}_1^{-1} \mathbf{x}_1 + \mathbf{S}_2^{-1} \mathbf{x}_2), \quad (\text{A3})$$

$$\mathbf{S} = (\mathbf{S}_1^{-1} + \mathbf{S}_2^{-1})^{-1} \quad (\text{A4})$$

If we now replace, in the above two equations,  $\mathbf{x}_1$  and  $\mathbf{S}_1$  by  $\mathbf{x}_a$  and  $\mathbf{S}_a$  (a priori estimates) and  $\mathbf{x}_2$  and  $\mathbf{S}_2$  by  $\hat{\mathbf{x}}_{LS}$  and  $\hat{\mathbf{S}}_{LS}$  above (based on a set of measurements  $\mathbf{y}$ ), we obtain

$$\hat{\mathbf{x}} = (\mathbf{S}_a^{-1} + \mathbf{K}^T \mathbf{E}^{-1} \mathbf{K})^{-1} (\mathbf{S}_a^{-1} \mathbf{x}_a + \mathbf{K}^T \mathbf{E}^{-1} \mathbf{y}) \quad (\text{A5})$$

$$\hat{\mathbf{S}} = (\mathbf{S}_a^{-1} + \mathbf{K}^T \mathbf{E}^{-1} \mathbf{K})^{-1} \quad (\text{A6})$$

This equation [see Rodgers, 1976] is the basis for the sequential estimation equations used in the MLS retrievals. Indeed, the above equations can be rewritten in a manner more similar to the "scalarized" equations (1) and (2) of section 3, namely,

$$\hat{x} = x_a + S_a K^T (K S_a K^T + E)^{-1} (y - y_a^c), \quad (A7)$$

$$\hat{S} = S_a - S_a K^T (K S_a K^T + E)^{-1} K S_a \quad (A8)$$

where departures from a priori state vector are now expressed as a function of departures from a priori radiances ( $y_a^c$ ).

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