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Validation of Tropospheric Emission Spectrometer (TES) measurements of the total, stratospheric, and tropospheric column abundance of ozone

G. B. Osterman,[1] S. S. Kulawik,[1] H. M. Worden,[1,2] N. A. D. Richards,[1,3] B. M. Fisher,[1] A. Eldering,[1] M. W. Shephard,[4] L. Froidevaux,[1] G. Labow,[5] M. Luo,[1] R. L. Herman,[1] K. W. Bowman,[1] and A. M. Thompson[6]

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[1] The Tropospheric Emission Spectrometer (TES) is an infrared, high-resolution Fourier transform spectrometer which was launched onboard NASA's Aura satellite in 2004 and is providing global, vertically resolved measurements of ozone in the troposphere. TES version 2 (V002) data profiles have been validated in the troposphere and lower stratosphere by way of comparison to ozonesondes and aircraft measurements. TES measurements also have sensitivity throughout the stratosphere, and therefore TES ozone profiles can be integrated to determine the total and stratospheric column in addition to the tropospheric column ozone values. In this work we compare the ozone in the stratosphere measured by TES to observations from the Microwave Limb Sounder (MLS) instrument in order to show the quality of the TES measurements in the stratosphere. We also compare the determination of a total column value for ozone based on the TES profiles to the column measured by the Ozone Monitoring Instrument (OMI). The TES tropospheric ozone column value is also calculated from the TES profiles and compared with column values determined from ozonesonde data. Column measurements are useful because the errors are markedly reduced from errors at the profile levels and can be used to assess both biases and quality of the TES ozone retrievals. TES observations of total or partial column ozone compare well with the other instruments but tend toward higher values than the other measurements. Specifically, TES is higher than OMI by $\sim$10 Dobson units (DU) for the total ozone column. TES measures higher values in the stratosphere (above 100 hPa) by $\sim$3 DU and measures higher ozone column values ($\sim$4 DU) in the troposphere than ozonesondes. While the strength of the TES nadir ozone product is the vertical resolution it provides in the troposphere, a tropospheric column value derived from TES have utility in analyses using or validating tropospheric ozone residual products.

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1. Introduction

[2] The Tropospheric Emission Spectrometer (TES) has been making measurement of ozone and other atmospheric constituents from the Aura satellite since late September 2004 [*Beer*, 2006]. TES measurements are sensitive to ozone in both the troposphere and stratosphere and therefore can be used to make an accurate determination of the total ozone column. TES measurements have undergone extensive validation; however TES sensitivity to ozone in the stratosphere has not been widely demonstrated. The study described in this work will provide a preliminary evaluation of TES ozone in the stratosphere. It will also illustrate the ability of TES to make an accurate determination of the total column value for ozone.

[3] This study will use Version 2 (V002) of the TES Level 2 data products. The previous Version 1 (V001) of the TES nadir ozone product has been preliminarily validated using ozonesondes [*H. M. Worden et al.*, 2007]. Version 2 of the TES data products represents a significant improvement over Version 1, primarily due to improved calibration of the

[1]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California, USA.
[2]Now at Atmospheric Chemistry Division, National Center for Atmospheric Research, Boulder, Colorado, USA.
[3]Now at Institute for Atmospheric Science, School of Earth and Environment, University of Leeds, Leeds, UK.
[4]Atmospheric and Environmental Research Inc., Lexington, Massachusetts, USA.
[5]Raytheon Technical Services Company, NASA Goddard Space Flight Center, Greenbelt, Maryland, USA.
[6]Department of Meteorology, Pennsylvania State University, University Park, Pennsylvania, USA.

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TES Level 1B radiances [*Shephard et al.*, 2008]. A description of the differences between the TES V001 and V002 Level 2 data products is available in the TES L2 Data User's Guide [*Osterman et al.*, 2007]. TES makes measurements in both the limb and nadir, but this study deals with validating only the nadir ozone data. The V002 TES nadir ozone products have been validated through an extensive analysis using ozonesondes [*Nassar et al.*, 2008; *Thompson et al.*, 2003, 2007] and aircraft lidar and in situ data [*Richards et al.*, 2008]. These analyses focused on the troposphere and lower stratosphere and show that in the lower and upper troposphere TES retrievals of ozone show a high bias compared to the ozonesondes and lidar measurements. Specifically, the TES ozone retrievals are higher than the ozonesondes by 2.9–10.6 ppbv in the upper troposphere and by 3.7–9.2 ppbv in the lower troposphere [*Nassar et al.*, 2008] while TES is higher than the lidar by 5–15% [*Richards et al.*, 2008]. The analysis described below is the first to focus on TES measurements in the stratosphere and examination of the total and tropospheric column ozone. In general, when comparing TES profiles with other measurements, it is essential to take into account the different sensitivities of the instruments by applying the TES averaging kernel. However, comparing columns rather than individual profiles significantly reduces the error due to averaging over pressure ranges larger than the TES vertical resolution. The total error for ozone columns averages 1.5%, as compared to 16.5% for the average profile error between altitudes 0 and 35 km. For this reason, we have decided to perform a simple comparison of ozone column products without accounting for the different instrument sensitivities.

[4] The Ozone Monitoring Instrument (OMI) also is operating from the Aura spacecraft. OMI measures backscattered solar radiance which allows it to measure column ozone as well as many other aerosol and chemical constituents of the atmosphere [*Levelt et al.*, 2006a, 2006b]. For the purposes of the study described here, we use the total ozone column data from OMI retrieved with the TOMS version 8 algorithm. OMI ozone column measurements have been validated by comparison to ground-based and other satellite observations [*Ziemke et al.*, 2006]. The OMI data are screened based on recommendations described at OMI Total Ozone (OMTO3) webpage at the Aura Validation Data Center http://avdc.gsfc.nasa.gov/Data/Aura/OMI/OMTO3/OMTO3_OVP_readme.html).

[5] The Microwave Limb Sounder (MLS) [*Waters et al.*, 2006] currently operates on the Aura spacecraft and measures the abundance of a large number of atmospheric constituents using measurements of thermal microwave limb emission. The ozone data used in this study are the MLS version 2.2, which has been validated for the upper troposphere and stratosphere in a number of studies [*Livesey et al.*, 2008; *Froidevaux et al.*, 2008; *Jiang et al.*, 2008]. The MLS Version 2.2 data quality document [*Livesey et al.*, 2007] provides information on properly flagging the MLS ozone products, and all MLS data shown in this analysis have been screened according to the specifications in that document.

[6] The analysis will focus first on TES/MLS and TES/OMI comparisons for a single "day" of TES data (actually ~26 hours) in July 2006. Then data from three time periods (January–March 2005, October 2005 and July 2006) will be used to understand the differences between column measurements made by the three Aura instruments.

2. TES Data and Ozone Retrieval Sensitivity

[7] The TES standard operating mode is called the global survey, which currently consists of a maximum of 3408 nadir measurements (scans) over approximately 26 hours (16 orbits). The nadir footprint is 5 km by 8 km [*Beer et al.*, 2001] and consecutive nadir profiles are separated by ~182 km for the current TES global survey. The definition of a TES global survey has changed since the instrument was launched; the original global survey had a maximum of 1152 nadir profiles as two nadir scans were averaged to produce a single profile. The original global survey also made routine limb measurements. In May of 2005 the global survey was changed to conserve instrument life, limb scans were removed and nadir scans were no longer averaged resulting in a maximum number of 3456 nadir profiles. In January 2006, the last sequence of each orbit was removed and replaced with an instrument maintenance measurement and the maximum number of profiles decreased to the current value of 3408. TES also makes special measurements that are used primarily for validation and important science opportunities. The TES L2 Data User's Guide [*Osterman et al.*, 2007] provides information on all TES measurement modes and their characteristics.

[8] The TES Level 2 data products provide extensive quality flag information to allow users to screen the data for good profiles. The TES Level 2 team has put together a main "master" quality flag to provide an initial recommendation as to the quality of a retrieved TES profile. All information necessary to recreate the master quality flag is provided in the data product file, so that a user can adjust the quality control criteria as needed [*Osterman et al.*, 2007]. Unless otherwise specified, the TES data used in this analysis include only data that have passed the "master" quality flag criteria.

[9] TES nadir retrievals provide profiles of ozone with vertical sensitivity that varies from scan to scan. The amount of vertical sensitivity varies with changes in the cloud properties of the observed footprint and the thermal properties of the atmosphere and Earth's surface. The best metric to understand the vertical sensitivity of a TES retrieved profile is the averaging kernel. The averaging kernel, which is provided in the data product for each TES scan, shows where the retrieved profile is sensitive and how the information gets smoothed through the profile [*Bowman et al.*, 2006; *H. M. Worden et al.*, 2007]. An example of a TES averaging kernel is provided in Figure 1 for a profile retrieved on 9 August 2006 over Baja, California. The TES sensitivity is spread over broad regions from 900 hPa up to nearly 1 hPa. This is a typical averaging kernel for northern midlatitude ozone retrievals and shows that TES has sensitivity over enough of the troposphere and stratosphere to give a good estimate of the total ozone column. In regions where the TES retrieved profiles are not sensitive, the TES averaging kernel will go to zero and values in the TES retrieved profile will revert back to their a priori value. The TES ozone and carbon monoxide a priori profiles are taken from climatology based on results from

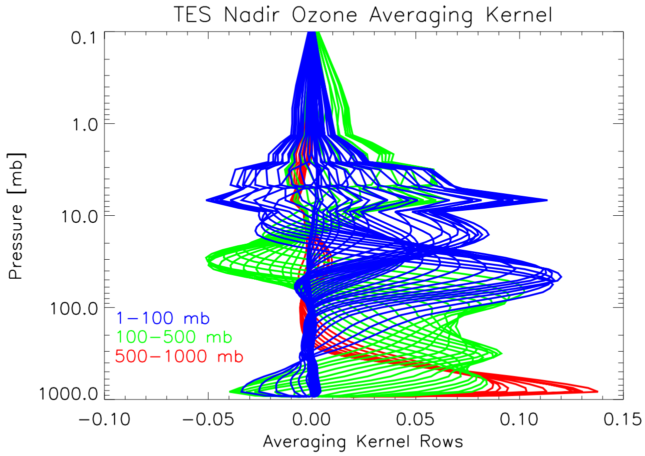

Figure 1. An example of a TES averaging kernel showing the locations of TES sensitivity in the atmosphere. The discontinuity at 10 hPa is due to a change to a coarser pressure grid in the TES retrieval process at higher altitudes.

the Model for OZone And Related chemical Tracers version 3 (MOZART 3) [*Brasseur et al.*, 1998] and calculated for use by the Aura instrument science teams (D. Kinnison, personal communication, 2003). The full MOZART climatology for ozone was reduced in spatial resolution to bins 10 degrees wide in latitude and 30 degrees wide in longitude. It is important to keep in mind when working with TES data that the reported profiles contain a mixture of regions where the measurement was sensitive to the chemical abundance in the atmosphere and regions where the retrieval has reverted back to the climatology. The averaging kernel is vital to understanding the locations of the sensitivity of TES data.

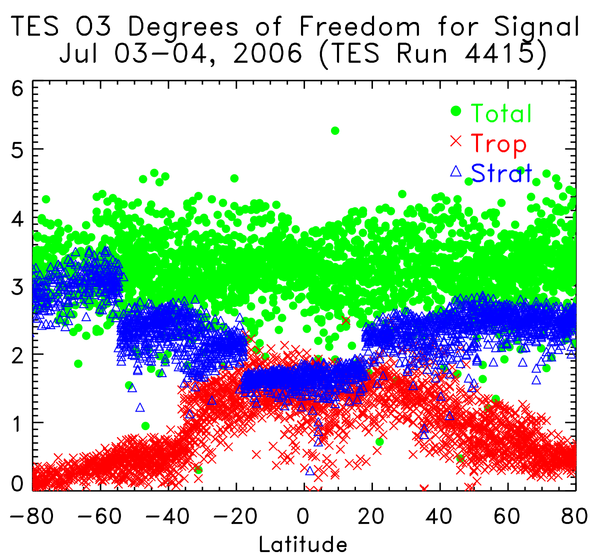

Figure 2. The TES degrees of freedom for the global survey of 3–4 July 2006. The blue data points show the number of pieces of information in the troposphere, while the red triangles show the dofs for the stratosphere. The discontinuities at 54°S, 18°S, 18°N, and 54°N are due to changes in the a priori constraint matrix used in the retrieval algorithm.

[10] The measure of the number of independent pieces of information in the TES retrieval is given by the degrees of freedom for signal (dofs) [*Rodgers*, 2000; J. *Worden et al.*, 2004]. The averaging kernel from Figure 1 has a dofs of 3.9. This means that there are nearly 4 pieces of information for the profile. The full-width–half-maximum of the averaging kernels in the troposphere determines the vertical resolution in the troposphere to be about 6 km. TES ozone profiles typically have 3 to 4 dofs, though the number can vary with cloud or surface conditions within the TES field of view. Figure 2 shows the degrees of freedom for signal for TES ozone measurements from a global survey taken on 3–4 July 2006. The sensitivity of the TES measurement to ozone in the troposphere and stratosphere will vary substantially for each retrieved profile. Figure 2 shows how the dofs in the troposphere for the ozone measurements is a maximum in the tropics and falls off with latitude toward the poles. It should be noted that because the dofs in the troposphere drops below one poleward of 45 degrees, TES will have little sensitivity to ozone as determined by the TES averaging kernel. It can also be seen

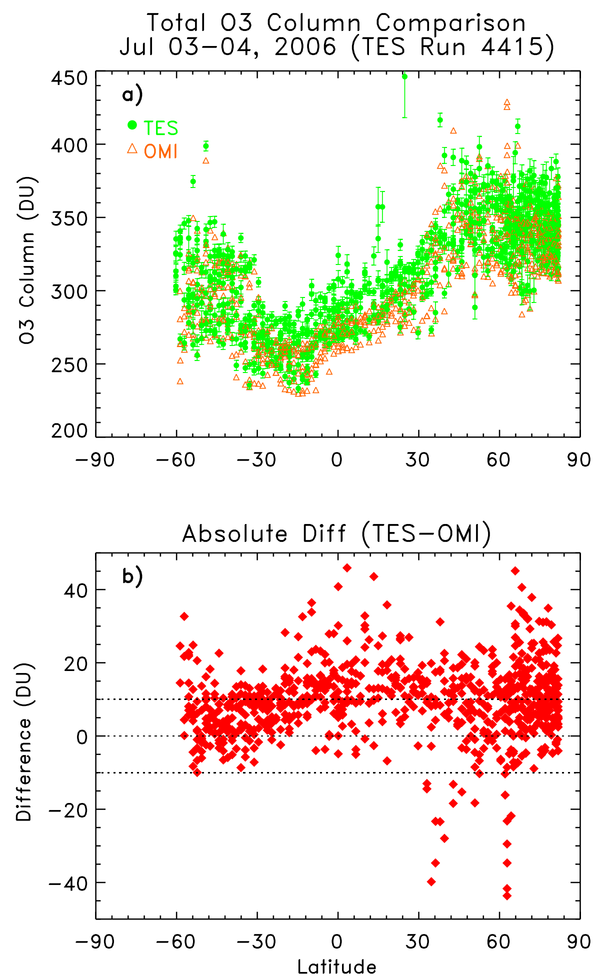

Figure 3. (a) TES and OMI total column ozone values for 3–4 July 2006 as a function of latitude. The error bars shown are the column error, as calculated using equation (3). (b) The absolute difference (in DU) between the TES and OMI measurements of the total ozone column as a function of latitude.

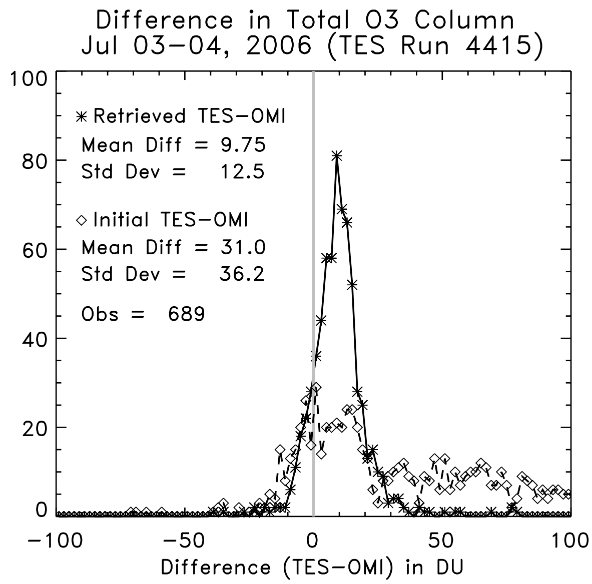

Figure 4. A histogram of the absolute difference between TES and OMI column ozone data. The histogram with the solid line (with asterisks) shows that TES retrieved values for the column are biased high by nearly 10 DU. The histogram with dashed line (with diamonds) shows difference calculated using the initial guess for the TES retrievals that are biased high with a large tail in the distribution at initial guess minus OMI greater than 30 DU. The improvement from the initial guess to the retrieved TES measurements suggests the TES retrieval is adding information and moving the data toward closer agreement with the OMI data.

that, outside the tropics, TES typically has at least 2 dofs in the stratosphere. The discontinuities seen in latitudinal distribution of the TES dofs are due to the a priori constraints used in performing the retrievals. The constraints are grouped by latitude into five (36°) bins. It is the ability of the TES ozone profiles to estimate the ozone in the stratosphere and ultimately determine a total column value that will be a prime focus of the analysis described here.

3. TES-OMI, TES-MLS Comparison for 3–4 July 2006

[11] TES values of the total ozone column are calculated using the logarithm of the retrieved ozone volume mixing ratio (VMR). The integration of the ozone profile uses log(VMR)/log(Pressure) interpolation of the profile between the TES levels (the same interpolation used in the TES retrieval process) and the TES reported air density and altitude for each profile. The column density (molecules/cm^2) can then be defined as:

$$\text{Column density} = \int VMR\rho dz = \sum_{layers} VMR_1\rho_1 \int_{z_1}^{z_2} e^{-\alpha_{VMR}(z-z_1)} e^{-\alpha_\rho(z-z_1)}, \quad (1)$$

where ρ is the air density, ρ_1 and VMR_1 are the values at the bottom of the layer, and α_{VMR} and α_ρ are the exponential decay of VMR and ρ, respectively. Here α_{VMR} can be solved in terms of VMR_1 and VMR_2, similarly for α_ρ. When the integral is integrated and evaluated at the layer boundaries, the equation for the column is

$$column = \sum_{layers} \frac{(x_1 - x_2)(z_2 - z_1)}{\ln(x_1/x_2)}, \quad (2)$$

where (1) values are for the level below the layer, (2) values are for the level above the layer $x = \frac{airdensity * O_3}{1 + H_2O}$ (where O_3 is the ozone VMR and the denominator uses the water VMR and converts to "dry" air density), and z = altitude. The error for the column, as discussed by *Kulawik et al.* [2006], can be calculated by using the chain rule. The reported error matrix for ln(VMR) is converted to an error covariance for VMR by multiplying by the VMR. The linear VMR error matrix is converted to a column error using the derivative of the column with

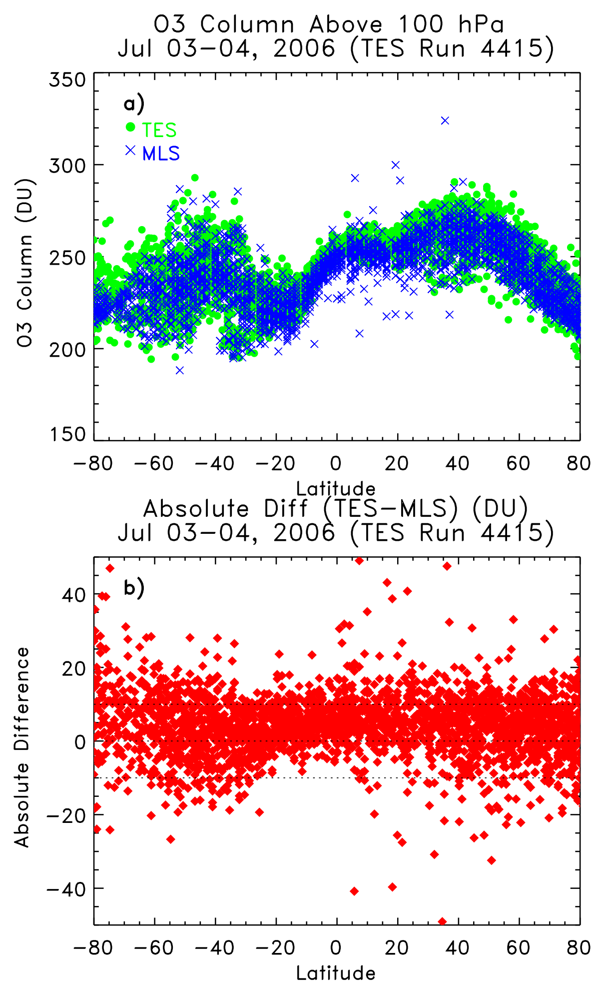

Figure 5. (a) The amount of ozone in the atmosphere above 100 hPa as determined by TES and MLS for measurements on 3–4 July 2006. (b) The absolute difference (in DU) between the TES and MLS values for the ozone column above 100 hPa.

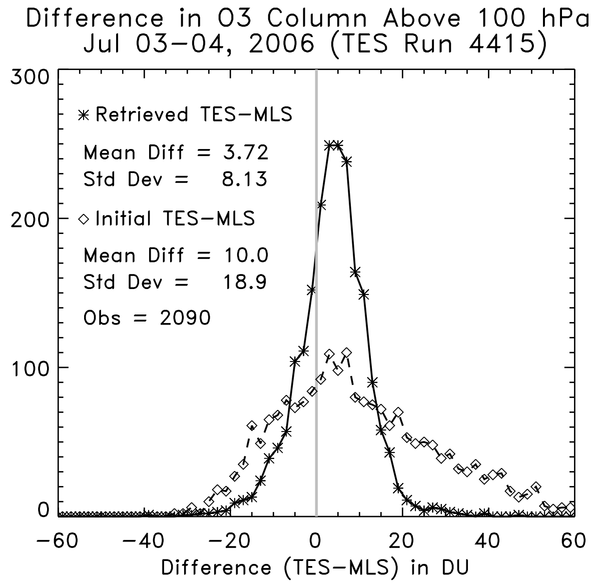

Figure 6. Similar to Figure 4, only showing the difference between TES and MLS column ozone above 100 hPa. The histogram with the solid line (with asterisks) shows that TES retrieved values for the column are biased high by nearly 4 DU. The histogram with dashed line (with diamonds) shows difference calculated using the initial guess for the TES retrievals that are biased by about 10 DU with a large tail. Again, TES ozone column shows significant improvement over the initial guess.

respect to the VMR for each level. The equation for the column error covariance is shown in equation (3),

$$S_{column} = \sum\nolimits_{i,j} VMR_i d_i S_{i,j} d_j VMR_j, \tag{3}$$

where d_i and d_j are the derivatives of the column with respect to the VMR at levels i and j, and $S_{i,j}$ is the error covariance matrix. This method was used for calculating all the column values described in this analysis. In the case of the TES tropospheric column values, discussed in a later section, the column values were created by integrating the TES reported profile up to the tropopause pressure provided in the NASA Goddard Space Flight Center Global Modeling and Assimilation Office (GMAO) GEOS-4 products (interpolated to the TES measurement location) [*Bloom et al.*, 2005].

[12] Typically, when comparing TES observations to other estimates of the chemical state of the atmosphere such as from ozonesondes, data from other satellite instruments or chemical model fields, the TES averaging kernel and a priori information must be taken into account [*Luo et al.*, 2007; *H. M. Worden et al.*, 2007]. These initial comparisons of the TES column values to those from OMI and MLS do not take the TES averaging kernel into account. The analysis is an attempt to provide a somewhat less rigorous estimation of the bias between the TES and OMI OMTO3 products. The ideal means of doing comparisons between TES and MLS profiles in the stratosphere would be to take into account the sensitivity of the two measurements [*Rodgers and Connor*, 2003]. This analysis provides users of TES data with preliminary information about the quality of TES ozone retrievals in the stratosphere by comparing column ozone amounts above 100 hPa with those calculated by MLS.

[13] Figure 3a shows TES column values calculated from ozone profiles measured during a global survey on 3–4 July 2006. Also plotted in Figure 3a are the OMI ozone column values for the same time period. The TES and OMI data were matched in time (scans less than 10 seconds apart) and distance (typically 7–10 km). Using only the nadir data from OMI allows for the best calculation of the absolute difference in the total column in Dobson units (DU) measured by the two instruments. The absolute difference between the matched TES and OMI nadir data is shown in

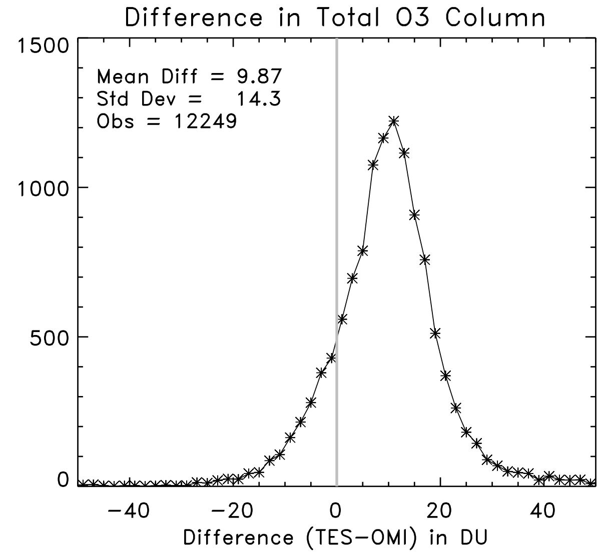

Figure 7. A histogram of the difference between TES and OMI for the January–March 2005, October 2005, and July 2006 data. TES is biased high by a value of 9.8 DU.

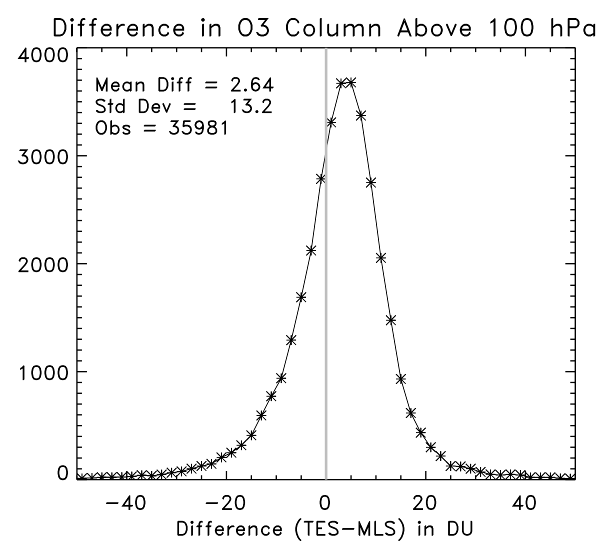

Figure 8. A histogram of the difference between TES and MLS for January–March 2005, October 2005, and July 2006 data. TES is biased high by a value of 2.6 DU in the stratosphere.

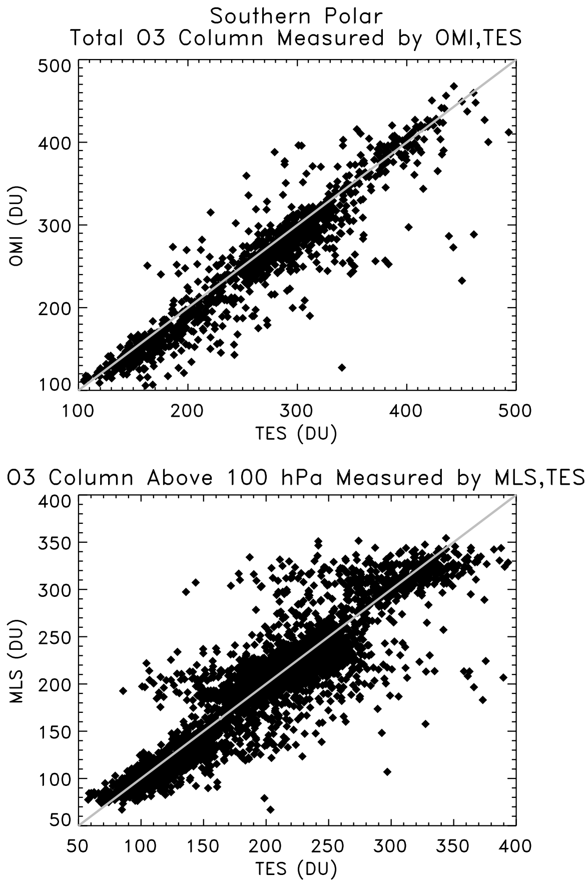

Figure 9. (top) Scatterplot of the TES and OMI total column ozone values from 11 TES global surveys worth of data from January–March 2005, October 2005, and July 2006. The plot shows only data from 60°N–82°N latitude. The correlation coefficient for this case is 0.9384. (bottom) A scatterplot for the TES and MLS ozone column values above 100 hPa for the northern polar region. The correlation coefficient for the TES, MLS data is 0.9331.

Figure 3b. The figure provides qualitative evidence of a high TES bias in the total column relative to OMI. The comparison for this particular global survey shows that TES column values are larger by roughly 10 DU (typically a percentage difference of between 2 and 5%, not shown) compared to OMI.

[14] Figure 4 shows a histogram of the absolute difference (TES-OMI) between the two instruments for all matched observations from the 3–4 July 2006 global survey. The data for this 26 hour period show a mean value for the (TES-OMI) difference of 9.7 DU with a standard deviation of 12.6 DU for 689 matched TES, OMI measurements. A histogram showing the difference between column values calculated from the TES initial guess profiles (instead of the retrieved profiles) and the matched OMI column values is given as the dashed line in Figure 4. The TES initial guess column has a high bias of 30.3 DU relative to OMI, with a large tail in the distribution at high values of ozone. There is significant improvement in TES ozone column retrievals relative to the initial guess (narrower distribution, smaller bias). This also indicates that anywhere in the TES retrieved profile where information is coming from the a priori (due to low sensitivity) that it will be positively biasing the TES reported retrieved profile, and thus total column values. Therefore, it is very likely at least part of the positive TES-OMI is attributed to the different sensor sensitivities, especially below ~900 hPa, and not due to retrieval errors.

[15] The data from MLS provide an excellent, thoroughly validated data set for evaluating TES measurements in the stratosphere. Calculating the column above 100 hPa insures that most of the comparisons will be of stratospheric air masses. The MLS stratospheric ozone columns (including those calculated for pressures above 100 hPa) have been validated using data from the SAGE II instrument and average difference between the two measurements is 0.5 DU [*Froidevaux et al.*, 2008]. The MLS ozone data have been compared to ozonesondes and agree to better than 1.3 DU at pressure levels at 100 hPa and above [*Jiang et al.*, 2008]. The MLS profiles were taken from v2.2 data files and quality controlled as spelled out in the MLS v2.2 Data Guide [*Livesey et al.*, 2007] and the TES and MLS scans closest in time

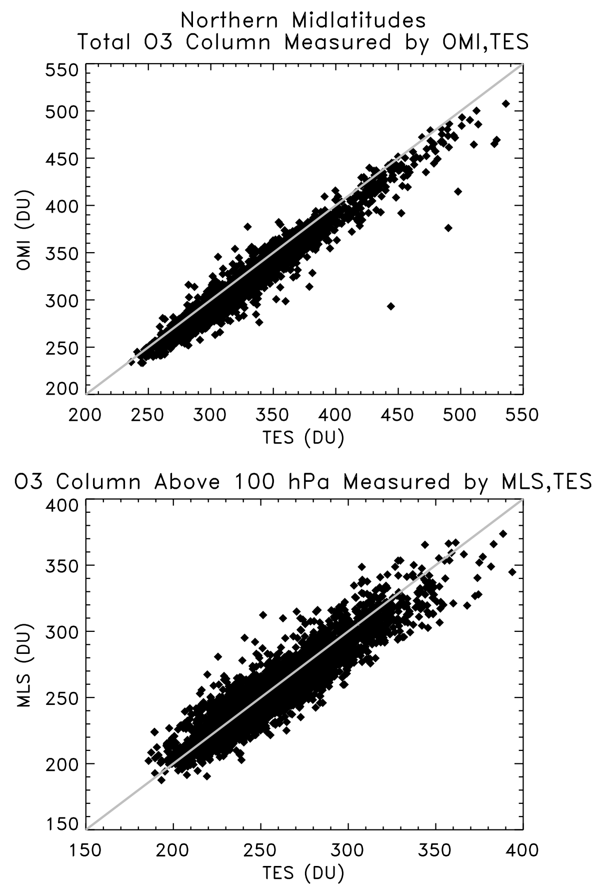

Figure 10. Similar to Figure 9. (top) A scatterplot of the TES and OMI total column ozone values from 11 TES global surveys worth of data from January–March 2005, October 2005, and July 2006. The plot shows only data from 30°N–60°N latitude. The correlation coefficient for this case is 0.9720. (bottom) A scatterplot for the TES and MLS ozone column values above 100 hPa for the northern midlatitude region. The correlation coefficient for the TES, MLS data is 0.9203.

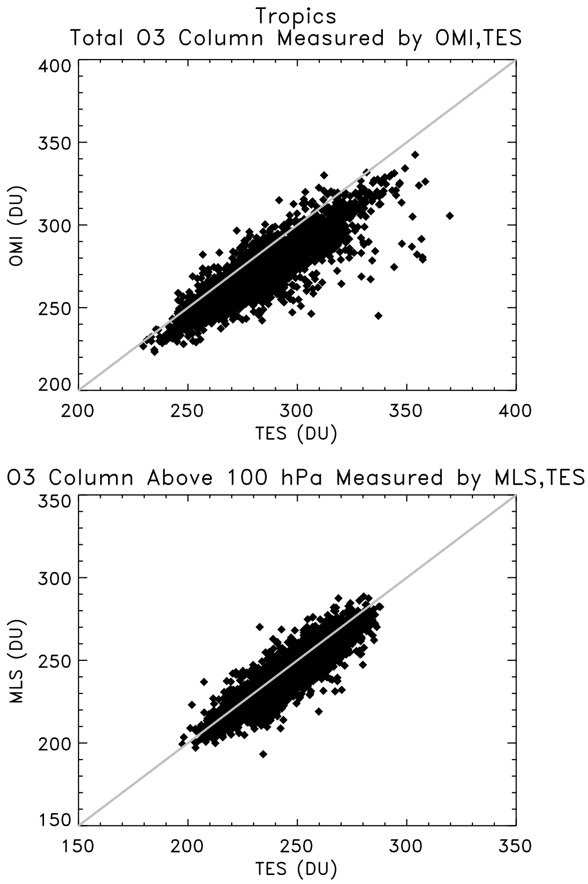

Figure 11. Similar to Figure 10. (top) A scatterplot of the TES and OMI total column ozone values from 11 TES global surveys worth of data from January–March 2005, October 2005, and July 2006. The plot shows only data from 30°N°N–30°S latitude. The correlation coefficient for this case is 0.8818. (bottom) A scatterplot for the TES and MLS ozone column values above 100 hPa for the tropical region. The correlation coefficient for the TES, MLS data is 0.9116.

and then distance were matched. The scans were typically made within 400–440 seconds of one another and the distance between the reported locations varied from 8 to 215 km. Figure 5a shows a comparison of the MLS and TES column ozone amount above 100 hPa for the 3–4 July 2006 global survey.

[16] The difference between the TES and MLS column values (in DU) above 100 hPa are provided in Figure 5b. Looking at the TES and MLS stratospheric column values (and their absolute difference) as a function of latitude there is no suggestion of either the clear high bias or the variations with latitude seen in the difference in the TES and OMI comparisons for 3–4 July. Figure 6 shows histograms similar to those in Figure 4 for the difference between the column above 100 hPa between TES and MLS (TES-MLS). Figure 6 shows that TES is biased high by 3.7 DU compared to MLS. Comparison of the TES initial guess column values above 100 hPa to MLS shows a mean bias of 10 DU with a standard deviation of 18.9 DU. The improvement in the bias (relative to MLS) from the TES initial guess to the retrieved column value in the stratosphere illustrates the sensitivity of TES retrievals to ozone above 100 hPa.

4. Data Comparisons for January–March 2005, October 2005, and July 2006

[17] The time periods January–March 2005, October 2005, and July 2006 provide a longer time period to examine the column ozone comparisons of TES to OMI and MLS. These time periods were selected because they were the longest periods during which all three satellite instruments had data available processed with the most recent version of the algorithms. The TES data are taken from 25 global surveys, during which nadir scans were averaged and the maximum number of scans was 1152 (January–March 2005), 3456 (October 2005) and 3408 (July 2006). The data from all the global surveys were screened for quality and matched with OMI data in a similar manner to that described in the previous section. Clouds are taken into account in the TES retrievals and are considered in the primary data quality flag that is provided with the

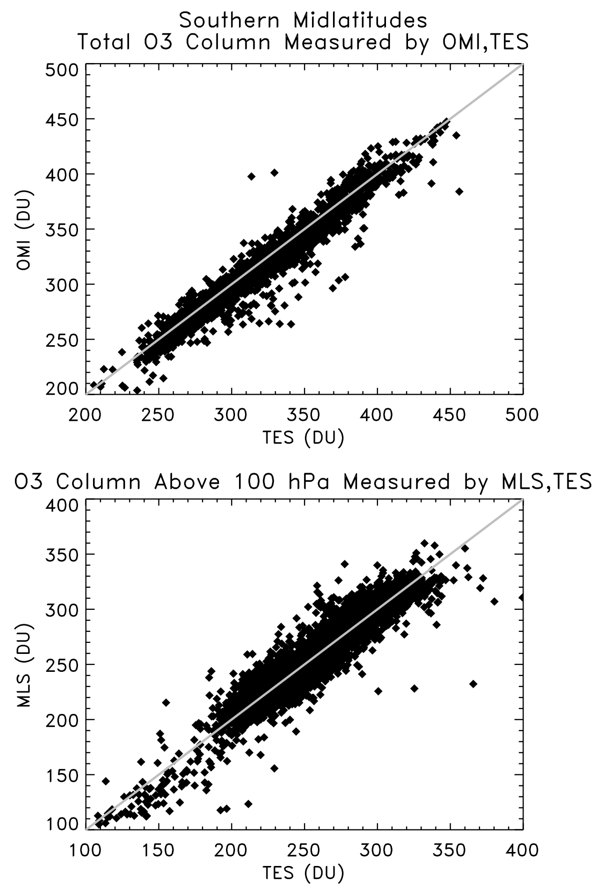

Figure 12. Similar to Figure 11. (top) A scatterplot of the TES and OMI total column ozone values from 11 TES global surveys worth of data from January–March 2005, October 2005, and July 2006. The plot shows only data from 30°S–60°S latitude. The correlation coefficient for this case is 0.9702. (bottom) A scatterplot for the TES and MLS ozone column values above 100 hPa for the southern midlatitude region. The correlation coefficient for the TES, MLS data is 0.9445.

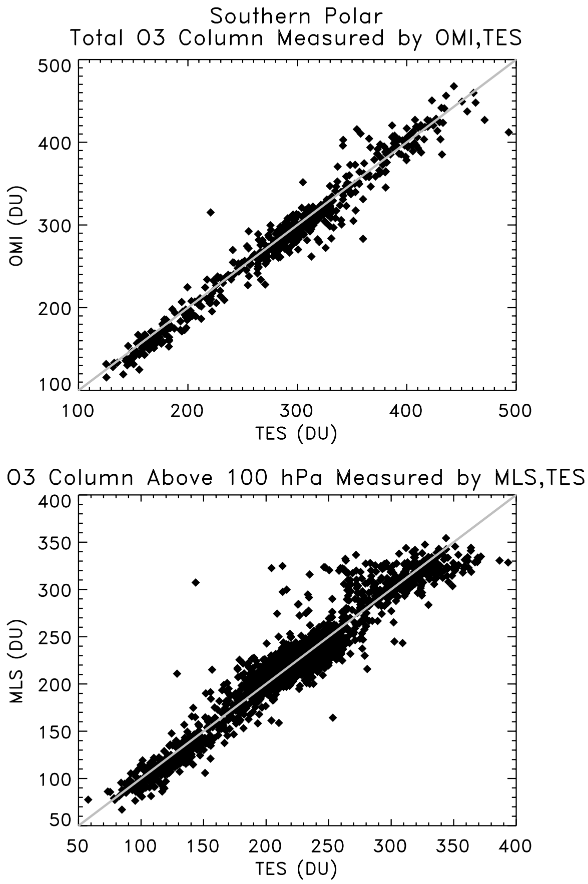

Figure 13. Similar to Figure 12. (top) A scatterplot of the TES and OMI total column ozone values from 11 TES global surveys worth of data from January–March 2005, October 2005, and July 2006. The plot shows only data from 60°S–82°S latitude. The correlation coefficient for this case is 0.9384. (bottom) A scatterplot for the TES and MLS ozone column values above 100 hPa for the southern polar region. The correlation coefficient for the TES, MLS data is 0.9595. In this case the data were further screened to include only TES measurements over ocean.

TES data products [*Osterman et al.*, 2007]. The clouds are accounted for in the retrieval by retrieving a series of frequency-dependent cloud parameters and has been shown to work well in the TES retrievals [*Kulawik et al.*, 2006; *Eldering et al.*, 2008], though it should be noted that the retrieval sensitivity is reduced below clouds. The difference in DU between the matched pairs was calculated and then averaged over the globe. The resulting mean bias is 9.84 DU as shown in Figure 7. The histogram result and the high bias of TES relative to OMI for the extended analysis time periods are very similar to the one calculated for a smaller sample in July 2006. The analysis from the previous section is repeated also for the comparison between MLS and TES column ozone above 100 hPa. The result as shown in Figure 8 is that TES is biased somewhat high relative to MLS in the stratosphere, similar to what was seen in the July 2006 global survey.

[18] Figures 9–13 are scatterplots between the matched TES, OMI and TES, MLS data binned between 60°N–82°N, 30°N–60°N, 30°N–30°S and 30°S–60°S respectively for the time periods of this analysis. In all cases the correlations between TES and the other Aura instruments are reasonably good. In the case of the Southern polar region (Figure 13) the data had to be further screened to include only ocean scenes. The retrieval of TES data over continental Antarctica is currently problematic and is under investigation and as a result we filtered the southern polar data to use only measurements over the ocean. The correlation coefficients for the comparisons from the combined time period data, as well as the bias and standard deviation for the quantities (TES-OMI) and (TES-MLS) are summarized in Tables 1 and 2. The results show that the column quantities calculated from the TES data correlate well with the quantities from OMI and MLS with TES biased high in all cases.

5. Determination of the Tropospheric Column

[19] MLS and OMI data products have been used together to generate tropospheric ozone residual (TOR) products [*Ziemke et al.*, 2006; *Schoeberl et al.*, 2008]. Given the extensive spatial coverage of OMI, these products provide excellent information about global distributions of tropospheric ozone. TES does not have the spatial coverage of these products but does provide vertically resolved information about ozone in the troposphere. However, TES can calculate a tropospheric column product that could be useful in comparisons with different TOR products and additionally provides sensitivity to ozone in troposphere that is complimentary to OMI [*Jourdain et al.*, 2007; *J. Worden et al.*, 2007]. Users of the TES tropospheric column data need to be aware that the retrieval process can smear information from the stratospheric true state into the troposphere, though the error incurred from this effect is included in the reported errors. The averaging kernel can be used to quantify the

Table 1. A Summary of the Bias, Standard Deviation, and Correlation of the TES Total Ozone Column Relative to the OMI Data for the Time Period January–March 2005, October 2005, and July 2006[a]

	Number of Data Points	Difference in the Total Column Ozone (TES-OMI)	Standard Deviation (TES-OMI)	Correlation Coefficient TES, OMI
All Latitudes	10,795	9.840	14.305	0.9645
60°N–82°N	1811	8.935	16.349	0.9384
30°N–60°N	2271	10.262	10.904	0.9720
30°N–30°S	4289	12.124	9.4495	0.8818
30°S–60°S	2424	5.393	10.902	0.9702
60°S–82°S	551	3.925	15.258	0.9384

[a]The difference and standard deviation values are in Dobson units.

Table 2. A Summary of the Bias, Standard Deviation, and Correlation of the TES Total Ozone Column Above 100 hPa Relative to the MLS Data for the Time Period January–March 2005, October 2005, and July 2006[a]

	Number of Data Points	Difference in Column Ozone Above 100 hPa (TES-MLS)	Standard Deviation (TES-MLS)	Correlation Coefficient TES, MLS
All Latitudes	35,267	2.644	13.212	0.9335
60°N–82°N	6443	0.928	11.203	0.9331
30°N–60°N	6632	3.313	9.923	0.9203
30°N–30°S	10,097	4.618	5.698	0.9116
30°S–60°S	7340	0.873	10.994	0.9445
60°S–82°S	2174	2.502	26.469	0.9595

[a]The difference and standard deviation values are in Dobson units.

average amount and impact of this smearing. Figure 1 illustrates this effect, the information in the pressure range 100–500 hPa clearly is spread from the stratosphere down into the troposphere for this particular Northern midlatitude profile. While the averaging kernel shown in Figure 1 is typical, the characteristics of the TES averaging kernel will vary with each measurement depending on factors such as cloud properties and the thermal contrast between the atmosphere and Earth's surface. Despite the fact that a tropospheric ozone column might contain some stratospheric information, there is enough information provided in the TES data to ensure the column provides useful information about the true atmospheric state.

[20] One way to provide an estimate of the quality of the TES tropospheric ozone column is to compare TES values to those calculated from ozonesonde data. Figure 14 shows a scatterplot of the ozone tropospheric ozone column values determined from TES profiles and those from coincident ozonesonde measurements including many launched specifically for TES overpasses (both day and night) [*Thompson et al.*, 2007]. Sonde data are taken from 32 ground stations around the world (latitude range 70°S to 80°N) with 1425 coincidences to TES observations between 11 October 2004 and 4 October 2006. The coincident criteria used was <9 hours and <300 km difference between the two measurements. The TES data are screened using both the master quality flag and additional criteria to remove instances of high ozone in the lower troposphere due to emission layers just above the Earth's surface [*Nassar et al.*, 2008] and all cloud cases are included in the comparisons. Also, the GMAO GEOS-4 value for the tropopause pressure was used for calculation of tropospheric column amounts from both the sonde and TES data. Typically comparisons between TES and ozonesonde profiles are done after application of the TES averaging kernel and a priori constraint [*H. M. Worden et al.*, 2007]. In this analysis, the tropospheric column ozone data were calculated from the sondes both before and after application of the TES averaging kernels. The column values calculated from the sonde data shown in Figures 14 and 15 are calculated without the application of the averaging kernel. The data plotted with black diamonds in Figure 14 show the correlation between TES and the sondes using coincidence criteria of 300 km and 9 hours between the measurements. The data plotted with the red diamonds in Figure 14 show the improved correlation that would be expected when the coincidence criteria are tightened to 100 km and 3 hours. The data in Figure 14 are for all latitudes and though not shown, there is no real difference in latitude in the correlation of the tropospheric column between TES and the sondes. Figure 15 is a histogram of the difference between the TES values for the tropospheric column ozone values and those obtained from the sonde data (without application of the TES averaging kernel). TES is seen to be biased high relative

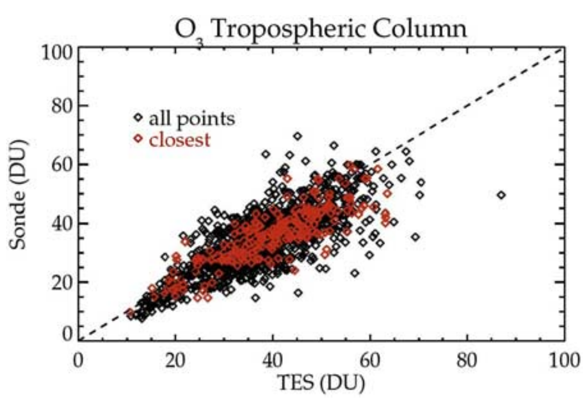

Figure 14. A scatterplot showing the TES "tropospheric column" compared to a column value calculated using ozonesondes. The black diamonds use coincidence criteria of 300 km and 9 hours, and the red diamonds use coincidence criteria of 100 km and 3 hours.

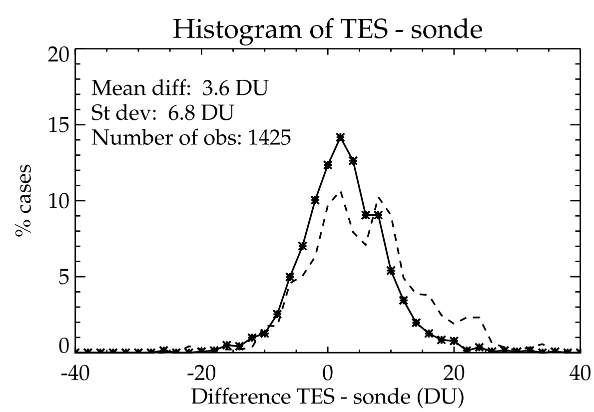

Figure 15. A histogram of the difference in the tropospheric column determined from profiles measured by TES and by ozonesonde. TES sees higher values of (on average) 3.6 DU. The dashed line is the difference using the TES initial guess.

Table 3. A Summary of the Bias and Standard Deviation of the TES Ozone Column in the Troposphere Compared to the Column Calculated From Ozonesondes[a]

	Difference in Tropospheric Ozone Column (TES-Sonde)	Standard Deviation in DU (TES-Sonde)
TES Initial Guess - Sonde	6.963	9.462
TES (without averaging kernel) - Sonde	3.631	6.783
TES (with averaging kernel) - Sonde	2.854	6.055

[a]The ozonesonde data used are global in their sampling and focus on cloud free scenes. The difference and standard deviation values are in Dobson units.

to the sonde by 3.6 DU. The finding that a high bias exists in TES relative to the sondes is consistent with the results of other validation studies involving TES v002 ozone measurements in the troposphere [*Nassar et al.*, 2008; *Richards et al.*, 2008]. The analysis shown in Figure 15 was repeated using the TES averaging kernels with the sonde data as described by *H. M. Worden et al.* [2007]. Comparison of the TES tropospheric column to that calculated from the sondes after the application of the TES averaging kernel reduced the bias to 2.9 DU in the tropospheric column with a 6.1 DU standard deviation. As expected, the application of the TES averaging kernel makes less difference for column comparisons than it does for profile comparisons owing to reduced smoothing error resulting from averaging and reduces the impact of the a priori in the comparisons. The tropospheric column calculated from the TES retrieved data clearly improves the TES-sonde bias over the TES a priori/initial guess with respect to the sondes as summarized in Table 3. The difference between the TES initial guess ozone column relative to the sondes is about 7 DU, while the difference between the TES retrieved values compared to the sondes is ~3.6 DU. The improvement in the standard deviation is from 9.5 DU to ~6 DU.

6. Conclusions

[21] Examining the global mean difference between the column values above 100 hPa determined by TES and MLS shows that TES is biased high by 3–5 DU. TES clearly improves on the a priori when compared to MLS, showing that in the column TES is clearly providing column information in the stratosphere. This is important since getting the stratosphere correct is vital for the ability of TES to properly estimate the ozone in the troposphere. TES does have sufficient sensitivity throughout the troposphere and stratosphere to measure a meaningful total column value for ozone. Comparisons of TES results with the OMI OMTO3 total ozone column product show that TES is biased high by 8–15 DU. There is considerable variability in the bias with latitude and this is still being studied. It is important to keep in mind that the sensitivity to ozone of the TES and OMI measurements will vary significantly with atmospheric pressure. Since the TES a priori profile has a ~30 DU total ozone positive bias with respect to OMI, it is very likely that some of the positive bias in the TES-OMI comparisons is attributed to the different sensor sensitivities and not TES retrieval errors, especially the contribution from below ~900 hPa where TES has low sensitivity. Finally, we show that the vertical information of the TES measurements in the troposphere allows for the calculation of a tropospheric ozone column which has a root-mean-square (rms) difference of 6 DU and bias of 3.6 DU compared to ozonesondes. This is a significant improvement over the initial guess and prior used by TES which has a 9.5 DU rms difference and a 7 DU bias. The high bias in the tropospheric column is consistent with the current understanding of a high bias in the tropospheric ozone profiles from TES compared to sondes. The analysis described in this paper provides an initial validation of TES tropospheric, stratospheric and total column ozone quantities, including the first validation of TES retrievals in the stratosphere. When this is coupled with the validation efforts of the TES tropospheric ozone profiles, we are able to make quantitative statements about the validation of the TES column.

[22] By the end of the year 2007, there will be enough of the newest TES data version (V003) and the MLS V2.2 data sets processed to provide an update to this analysis and to better quantify the bias of TES relative to MLS in the stratosphere as a function of season and latitude. Comparisons of TES data to ozonesondes [*Nassar et al.*, 2008] suggest that TES is biased high in the lower stratosphere and a summary of the sonde comparisons in this region will be included in a future analysis. Similarly, more statistics about the seasonal and latitudinal variations in the high bias in the total ozone column observed by TES relative to OMI will be provided. Finally an analysis to better quantify how the different sensitivities of OMI and TES affect the observed biases will be performed.

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K. W. Bowman, A. Eldering, B. M. Fisher, L. Froidevaux, L. Herman, S. S. Kulawik, M. Luo, and G. B. Osterman, Jet Propulsion Laboratory, California Institute of Technology, MS 183-601, 4800 Oak Grove Drive, Pasadena, CA 91109, USA. (gregory.osterman@jpl.nasa.gov)

G. Labow, Information Technology and Scientific Services, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, USA.

N. A. D. Richards, Institute for Atmospheric Science, School of Earth and Environment, University of Leeds, Environment Building, Leeds LS2 9JT, UK.

M. W. Shephard, Atmospheric and Environmental Research Inc. (AER), 131 Hartwell Avenue, Lexington, MA 02421, USA.

A. M. Thompson, Department of Meteorology, Pennsylvania State University, 510 Walker Building, University Park, PA 16802, USA.

H. M. Worden, Atmospheric Chemistry Division, National Center for Atmospheric Research, P.O. Box 3000, Boulder, CO 80305-3000, USA.