Aura-TES L2 Products: Version 4 Quality Description

Overview of Current Data Quality Status

The TES data products have undergone significant validation analyses. The L2 data nadir products ozone, carbon monoxide, water vapor, temperature, HDO and sea surface temperature are all validated and usable in scientific analyses. Details on the validation of the latest version of TES data version (V004, F05_05/F05_06/F05_07) will be available in an updated TES Validation Report in late 2009 (Osterman et al., 2009). The current validation report (V003 and V002 data) is available on the Langley ASDC web site and the TES web site. This document will be updated in a new version of the Data User's Guide when the updated validation report is available in late 2009. A full description of the TES V002 L1B data product quality is available. The subsections below give an overview of the validation and data quality analysis of TES V004 data and/or on the quality of earlier versions of the TES data products.

There also have been 13 papers published in a special issue of Journal of Geophysical Research Atmospheres dealing with Aura validation published in 2008. The validation papers and other TES publications are available at the TES publications web site.

Data Quality and Validation Status for TES Level 2 Data Products

Nadir Ozone

The most complete validation analysis of TES nadir ozone retrievals was done using the V002 data set. A statistical comparison of the V002 TES ozone profiles to ozonesondes shows that TES has a high bias of 3-10 (5-15%) ppbv in the troposphere (Nassar et al., 2008). In particular, the bias in the lower troposphere ranges from 3.7-9.2 ppbv while in the upper troposphere the range is 2.9-10.6 ppbv. The linearity in the correlation of the sonde and TES data provide confidence in the ability of TES to pick up variations in ozone in the troposphere. Comparisons of TES data to measurements from the National Aeronautics and Space Administration (NASA) Langley Research Center Differential Absorption Lidar (DIAL) instrument show a similar high bias in the troposphere of between 5-15% (Richards et al., 2008) in measurements made during the Spring, 2006 over the Pacific Ocean, North America and the Gulf of Mexico. Comparisons of stratospheric ozone columns calculated from the TES data to similar columns from Microwave Limb Sounder (MLS) ozone show good agreement with TES biased high by 2-5 Dobson Units (DU) (Osterman et al., 2008).

An analysis showing comparisons of ozonesondes to the TES V003 nadir ozone data show a similar high bias in the TES profiles when properly screening the data for good retrievals. The latest TES data version, V004, is only partially processed as of May 2009. Comparisons of the V004 retrievals to sondes show similar results to previous data versions, a 5-15% high bias in the TES data compared to sondes. A thorough global reanalysis of the TES ozone profiles and how they compare to ozonesondes is expected to be completed in late 2009 as the V004 data are processed for the entire TES data record.

Nadir Carbon Monoxide

Validation analyses of TES carbon monoxide V002 and V003 data products have been documented in the TES validation report (Osterman et al., 2007) and validation publications (Luo et al., 2007a; Luo et al., 2007b; Lopez et al., 2008). Few differences are found between TES V002 and V003 CO fields for the tropics and mid-latitudes. The major difference between the two versions is the larger variability seen in the V003 data at high latitudes due to relaxation of the *a priori* constraints.

Comparisons have been carried out between TES carbon monoxide retrievals and those from a variety of satellite and aircraft instruments. Global patterns of carbon monoxide as measured by TES are in good qualitative agreement with those seen by Measurement of Pollution in The Troposphere (MOPITT) on the NASA Terra satellite. Comparisons of profiles of CO between TES and MOPITT show good agreement when a priori information is accounted for correctly. TES carbon monoxide agrees to within the estimated uncertainty of the aircraft instruments, including both errors and the variability of CO itself. TES V004 CO data values do not show systematic changes from V003 or V002 with increased number of good quality retrieved profiles. One difference between the V003 and V002 occurs at high latitudes where the V003 data is the larger variability seen in the V003 data at high latitudes due to relaxation of the *a priori* constraints. This would occur with V004 data as well.

Comparisons to the aircraft in-situ measurements during International Chemical Transport Experiment (INTEX-B) 2006, Aura Validation Experiment (AVE) (Houston, TX) 2004, CR-AVE (San Jose, Costa Rica) 2006, and Polar Aura Validation Experiment (PAVE) 2006 are performed to help assess the TES CO retrieval accuracy and to address the influences of tracer spatial/temporal variability to the comparisons. The agreement between TES CO profiles and data taken *in situ* is typically within 15%, less than the variability of the CO in TES and aircraft measurements. Lopez et al. (2008) reported that, in the 700-200 hPa pressure range where TES is sensitive to CO, in-situ measurements from the WB-57 aircraft agree with TES to within 5-10%.

Global comparisons between Terra MOPITT and TES CO measurements have been performed as well. The results show that for pressure layers where both instruments are most sensitive, the retrievals agree to within 10%. The global CO pattern observed by TES shows similar qualitative features to those seen by MOPITT. Comparison between TES CO data in the upper troposphere and those from the ACE instrument show an agreement of 7.4% at 316 hPa.

In early December 2005, an adjustment was made to the optical bench temperature that improved the quality of the TES CO product. Data taken after December 6, 2005 are of better precision and have better vertical resolution.

Nadir Atmospheric Temperature

The newly available TES version 4 (v004) data feature improvements that significantly impact nadir temperature retrievals. Improvements were made to the forward model, retrieval strategy, constraints, and climatology (Herman et al., 2009; Shephard et al., 2008b). TES v004 temperature retrievals have been compared with nearly coincident radiosonde (hereafter sonde) measurements from the NCEP database for temperature bias analysis. The bias in the TES nadir temperature retrievals is significantly reduced in v004 to <0.7 K, compared with a 1 to 2 K upper tropospheric cold bias in v003. Here is a breakdown of the bias with different criteria:

- bias over ocean is <0.6 K (531 TES-sonde matches)
- bias over land is <0.5 K (1118 matches)

TES nadir temperature retrievals were also compared with the NOAA ESRL database for analysis of temperature rms. This database provides a better estimate of rms because exact sonde launch times are known, which allows a closer match in time to the TES retrieval. The TES temperature rms in v004 is 1 K in the stratosphere and upper troposphere and 1.5 K in the lower troposphere (at 500 to 900 hPa), compared to 2-4 K in v003. There is an uncertainty of 0.5 to 1 K simply due to the spatial and temporal variability of atmospheric temperature.

Nadir Water Vapor

Retrievals of water from TES show a wet bias throughout much of the troposphere when compared with the Cryogenic Frostpoint Hygrometer (CFH) and RS90/RS92 radiosondes, both globally (NCEP sonde database) and in detailed comparisons (validation field missions). The most detailed comparisons come from the Water Vapor Validation Experiments (WAVES_2006) carried out at Beltsville, Maryland. WAVES_2006 had coordinated water vapor observations by lidar, CFH, and RS92 radiosondes timed with TES transect special observations. The TES bias relative to CFH is on the order of 5-10 % below 700 hPa and 5-40% between 700 and 300 hPa (Shephard et al., 2008b). Definitive conclusions from the comparisons are difficult to obtain because of sampling issues, differences in sonde measurements and the extreme inherent variability of water in the troposphere. Shephard et al. (2008b) carried out a radiance closure study based on the WAVES_2006 comparisons, and concluded that estimated systematic errors from the forward model, TES, in-situ water and temperature measurements, and clouds are not large enough to explain the observed differences between TES and CFH. He concluded that either there are unaccounted systematic errors, or a sampling mismatch. The differences seen between TES and the sondes were fairly consistent for both V002 and V003 data. The TES water profiles have shown good qualitative agreement with in situ aircraft data from PAVE 2006 and AVE field missions. Comparisons of TES V002 data and AIRS total column water vapor is 10% drier than Advanced Microwave Scanning Radiometer (AMSR-E) and AIRS. Comparison of the water vapor profiles from TES and AIRS show that most of the difference in the column is accounted for by the 700-900 hPa layer.

Nadir HDO

Comparisons of the TES HDO/H2O ratio to models, to the expected HDO/H2O ratio over oceans and to aircraft observations in the lower troposphere suggest that the HDO/H2O ratio is 5% too high. This bias is likely associated with either the H2O or HDO spectroscopy (or both) and/or with the TES calibration. Future co-located observations of in-situ observations will allow us to better understand this bias.

Because the problem of estimating HDO is highly non-linear, it is suggested that the data only be used when the sensitivity, as defined by the "DegreesOfFreedomForSignal" variable in the product files has a value of 0.5 or higher. This is an ad-hoc threshold based on current analysis of the data and may be adjusted in the future.

Nadir Methane

TES V004 methane has been compared with in-situ aircraft measurements from the Differential Absorption CO measurement (DACOM) instrument for flights during the INTEX-B campaign, with satellite measurements from AIRS (on the Aqua satellite) and with global monthly fields from GEOS-Chem, a global chemical model which has previously been shown to compare well with a range of ground-based and aircraft measurements. Preliminary comparisons have also been performed against data from ground-based FTIR instruments maintained by the Network for the Detection of Atmospheric Composition Change (NDACC).

TES methane retrievals contain around 1.0 degree of freedom for signal (DOFS) - between ~0.5 in Polar Regions and 1.4-1.8 in the tropics, depending on season and location. With only one degree of freedom available, attempts to interpret TES methane (or differences between TES methane and some other data source such as model fields or in situ data) on any given one of the 67 Level 2 levels can be misleading. Since methane is relatively well-mixed in the troposphere, the TES methane may be represented by a representative tropospheric volume mixing ratio (RTVMR), associated with an effective pressure that describes the location in the atmosphere where most of the retrieval information originates. Further discussion of this quantity can be found in V. Payne et al., (2009) published in the Journal of Geophysical Research - Atmospheres.

Nadir Surface Temperature (Sea Surface Temperature)

TES retrieves surface (skin) temperature as standard product. Over ocean this amounts to a sea surface temperature (SST). Comparisons of TES V003 data to the Reynolds Optimally Interpolated (ROI) sea surface temperature product between January 2005 and July 2008 show very small biases. The TES V003 observations have a bias relative to ROI data for night/day of -0.20/0.04 K. A full analysis of the TES sea surface temperature product will be completed Fall 2009 as more of the V004 data set finishes back processing. The validation analysis performed to date suggests the TES measurements of sea surface temperature are robust and are a good marker for the stability of the TES

radiances.

TES Nadir Cloud Products

Cloud products were validated by comparing TES estimates of effective cloud optical depth and cloud top height to those from the Moderate Resolution Imaging Spectroradiometer (on EOS) (MODIS), the Atmospheric Infrared Sounder (AIRS), and to simulated data. The radiance contribution of clouds is parameterized in TES retrievals in terms of a set of frequency-dependent nonscattering effective optical depths and a cloud height. This unique approach jointly retrieves cloud parameters with surface temperature, emissivity, atmospheric temperature, and trace gases such as ozone from TES spectral radiances. We calculate the relationship between the true optical depth and the TES effective optical depth for a range of single-scatter albedo and phase functions to show how this varies with cloud type. We estimate the errors on retrieved cloud parameters using a simulated data set covering a wide range of cloud cases. For simulations with no noise on the radiances, cloud height errors are less than 30 hPa, and effective optical depth follows expected behavior for input optical depths of less than 3. When random noise is included on the radiances, and atmospheric variables are included in the retrieval, cloud height errors are approximately 200 hPa, and the estimated effective optical depth has sensitivity between optical depths of 0.3 and 10. The estimated errors from simulation are consistent with differences between TES and cloud top heights and optical depth from MODIS and AIRS.

Limb Ozone

Comparisons of the TES limb ozone compares well to TES nadir ozone when the averaging kernel is considered in the comparisons. On average, the limb retrievals are biased high when compared to both the TES nadir retrieval and to data from the Microwave Limb Sounder (MLS) also on the Aura satellite. In the V004 data, TES limb ozone has a high bias of 10-15% in the lower stratosphere. The bias increases to 15-35% in the upper stratosphere. The magnitude of the bias is lower in the V003 data, but changes in the manner in which clouds are detected in the V004 retrievals allow for data sensitivity into the upper troposphere. The validation analysis is very preliminary.

Limb Atmospheric Temperature

TES version 4 (v004) limb temperature retrievals have improvements over earlier versions. Improvements were made to the forward model, retrieval strategy, constraints, and CO2 climatology, as described in more detail in the nadir temperature validation section of the TES Validation Report (Osterman et al., 2009). In the first statistical comparison between TES v004 limb temperature and radiosondes, TES is typically within 0.5 K of radiosondes in the troposphere, with a -0.7 K cold bias at 40 to 50 hPa in the lower stratosphere, and a warm bias > 1 K in the middle stratosphere. The rms is typically 2 K.

Limb Nitric Acid

Limb nitric acid has been compared to data from in situ aircraft instruments, aircraft Fourier Transform Infrared (FTIR) and other satellite instruments such as EOS MLS. V004 nitric acid has more sensitivity to the upper troposphere due to an increased threshold for cloud detection, allowing the inclusion of data from more tropospheric detectors. Comparisons to Chemical Ionization Mass Spectrometer (CIMS), the University of New Hampshire (UNH) Soluble Acidic Gases and Aerosols (SAGA) instrument, and results from the Microwave Limb Sounder (MLS) indicate TES HNO3 results are reasonable between 10 and 260 hPa with about a 30% uncertainty and no known bias.

Limb Water Vapor

TES v004 limb water vapor is an interfering species in the retrieval of limb O3 and HNO3. Limited analysis of the limb water product shows low sensitivity.