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Aura-TES L2 Products: Version 6 Data Quality Description

Overview of Current Data Quality Status

This is a preliminary report on data quality of TES Version 6 data (Version 6, files ending in F07_10). For water vapor and atmospheric temperature initial guess and constraint, the Global Modeling and Data Assimilation Office (GMAO) GEOS-5.9.1 model is used. Due to limited availability of GEOS-5.9.1, it is not possible at the time of this publication to fully assess the validation or data quality of TES Version 6. Previous versions of the TES data products have undergone significant validation analyses. Version 5 Level 2 data nadir products ozone, carbon monoxide, carbon dioxide, water vapor, temperature, HDO, sea surface temperature, methane and ammonia are all validated and usable in scientific analyses. Details on the validation of Version 5 TES data (V005, F06_08 and F06_09) are available in the TES Version 5 Validation Report (Herman et al., 2012), including Version 5 L1B radiances.

The subsections below give a brief overview of the latest data quality analysis of TES Version 6 and/or Version 5 data. In order to successfully interpret TES data one must account for the variable vertical sensitivity of the TES product and the *a priori* constraints used to help convert measured radiances to vertical profiles of tropospheric composition. Biases in the data can also vary with altitude. Comparisons between TES data and earth atmosphere models can also be challenging because of possible logarithmic differences between the data product, *a priori*, and model fields.

We therefore recommend that the scientist interested in TES data read Chapter 9 of the TES Data User's Guide (Herman et al., 2013) on how to interpret and use TES data and any published papers in which the data are used (all published papers using TES data are listed on the TES website). For example, these papers will discuss how biases are addressed or how logarithmic differences between TES data and model fields affect scientific interpretation. All of the TES validation papers and other publications are available at the TES publications web site.

Users should also read the quality statement listed below. For most scientific applications a data user should select data using the master data quality flag ("speciesretrievalquality") and a check on the sensitivity with the DegreesOfFreedomForSignal data field. If these checks are removing too much data over the area of interest then the user should contact a member of the TES science team on how to use a subset of flags.

Data Quality and Validation Status for TES Level 1B Radiance Data Product

Though this report is focused primarily on the TES Level 2 data products, it is important to understand that the L1B radiance products have also undergone a rigorous validation as reported

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in Shephard et al. (2008) and in the TES Validation Report V003 (Osterman et al., 2007). The fundamental measurement of the Tropospheric Emission Spectrometer (TES) on board the Aura spacecraft is upwelling infrared spectral radiances. Accurate radiances are critical for trace gas profile retrievals for air quality as well as sensitivity to climate processes. For example, any radiometric systematic errors (*e.g.* calibration) not addressed in the L1B radiances will propagate as errors into the retrieved atmospheric parameters (Bowman et al., 2006; Worden et al., 2004). Connor et al (2011) showed that the TES relative radiometric calibration was extremely stable over the time period used in their analysis: 2005 to 2009.

A new product in TES Version 6 related to radiance is the ozone band radiative flux, specifically FM ozone band flux and L1B ozone band flux. These both have units of W/m^2 and represent the TOA flux for the ozone band from 985-1080 cm^{-1}, as measured by TES (L1B) and as estimated by the radiative transfer forward model (FM) at the convergence of the L2 retrieval. The flux values were computed using the anisotropy estimate described in H. Worden et al., (2011). Both L1B and FM flux variables have reasonable values as a function of latitude, and comparing all-sky and clear-sky. Differences between L1B and FM fluxes are consistent with radiance residuals close to measurement noise. A comparison was carried out between TES ozone band fluxes and 10° latitude bins of IASI flux values for 15 Aug 2008. IASI radiances are nominally cloud free (< 25% cloud filled pixels) and here we used scans that are closest to nadir (|sat ZA| <10°), including day/night, land/ocean. For the IASI comparison, we assumed a single value for anisotropy = 1.1 (the number in H. Worden et al., 2011 for the ozone band in cloud-free ocean scenes). For histograms of IASI ozone band flux values by latitude band, the distributions have peaks close to the TES values for clear sky at the corresponding latitude, as expected.

In April 2010, TES implemented a new strategy for observing and processing calibration measurements (see Section 4 of the Version 5 Data Validation Report, Herman et al., 2012). In order to validate TES spectra processed with the new calibration strategy, and to check comparisons of TES with AIRS over the entire TES data record from 2004 to present, we developed a more automated comparison tool based on the methods used for TES/AIRS comparisons in Shephard et al. (2008). Given the differences in ground footprints for TES and AIRS, comparisons are only meaningful for clear-sky, ocean scenes. Results for April 2009 (old calibration approach) compared to April 2010 (new calibration approach) are not significantly different, which suggests the new approach provides the same radiance accuracy as before.

Data Quality and Validation Status for TES Level 2 Data Products

Nadir Ozone

The retrieval algorithm of TES Version 6 ozone profiles is nearly identical to that of Versions 5 and 4. A new ozone climatology is used as initial guess for Version 6 ozone. The Version 6 TES ozone product quality flags are too strict, *e.g.*, good profiles are flagged bad. This issue will be addressed in the upcoming months, but in the meantime the user is recommended to contact the TES Science Team on how to use a subset of the quality flags. The TES Version 5 validation report (Herman et al., 2012) showed that the percent and absolute biases of TES-sonde are congruent to previous validation studies of TES V001 and V002. TES nadir ozone profiles provide data that were measured in the TES global survey, step-and-stare, transect, and stare

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observation modes. These have been compared with a subset of ozonesonde measurements from ARCIONS (Canada) and a global ozonesonde database. Coincidence criteria of ±9 h, 300-km distance and a cloud optical depth less than 2.0 were applied to search for the TES-ozonesonde coincidence measurements. Flagged TES data were filtered out. For the limited number of processed TES validation runs, we find that the 1-sigma standard deviation of TES-ozonesonde differences is nearly identical between Versions 5 and 6. One TES global survey (runid 10310) was randomly selected to compare Versions 5 and 6. We find nearly identical throughput, and similar mean bias. These features are consistent with that of Boxe et al. (2010) and TES Version 5 Validation Report (Herman et al., 2012).

Nadir Carbon Monoxide

TES CO Version 6 data are very similar to Version 5 data. This is expected since neither retrieval algorithms nor operational support data related to CO retrievals are updated in Version 6. The mean difference in CO volume mixing ratio comparing two version data globally is less than 1%, with standard deviation of a few percent. This very small change is due to changes in temperature and other interfering species.

Version 5 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 MOPITT on the NASA Terra satellite. Comparisons of profiles of CO between TES and MOPITT show better 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. In the upper troposphere, TES CO are found to bias lower compared to that of MOPITT by a few percent.

Nadir Carbon Dioxide

TES CO_2 is retrieved between 40 S and 45 N, with average cloud optical depth < 0.5, among other tests, for good quality. On average, TES CO_2 has an average of 0.65 degree of freedom for signal (DOFS) – with the most DOFS for daytime land cases (which can be on the order of 1 DOFS) and the least for nighttime or winter land cases (which can be on the order of 0.3 DOFS). Ocean targets (day or night) have intermediate DOFS with about 0.8 DOFS. The averaging kernel indicates sensitivity between the surface to above 100 mb, with the most sensitivity between about 700 and 300 mb, peaking at about 600 mb. Although a profile is retrieved and has been validated, there is very little independent information at the different profile levels and it is critical to utilize the provided averaging kernel when using TES data. TES Version 6 CO_2 has been compared with aircraft vertical profiles over the Pacific from the HIAPER (High-Performance Instrumented Airborne Platform for Environmental Research) Pole-to-Pole Observation (HIPPO) program (Wofsy et al., 2011) and shows modest improvements over Version 5 results. The Version 5 quality statement applies for now with some improvement in accuracy noted in the Version 6 validation datasets that have completed so far. Further details of Version 5 validation can be found in Kulawik et al. (2012).

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Nadir Atmospheric Temperature

TES Versions 5 and 6 nadir temperature (TATM) retrievals have been compared with nearly coincident radiosonde (hereafter sonde) measurements from the NOAA ESRL global sonde database. For TES Version 6 TATM relative to radiosonde (with averaging kernel applied), the mean bias is +0.5 K in the lower troposphere, -0.5 K in the upper troposphere. This is similar to Version 5 comparisons. The rms is less than 1 K in the stratosphere and upper troposphere, but increases to 1.7 K in the lower troposphere.

To evaluate the retrieval stability the monthly mean and standard deviation of the TATM residual between TES Version 5 and the Global Modeling and Data Assimilation Office (GMAO) GEOS-5 model, which provides the first guess and a priori for the TATM retrieval, were calculated. The statistics for both Tropical Pacific and Northern Atlantic Ocean regions indicate only minor month-to-month variability and no substantial trends over the entire five-and-a-half year period. The standard deviation of the residual was generally smaller than the standard deviation of the GMAO GEOS-5 but larger than the TES estimated measurement error. Overall, based on this analysis it appears that the TES retrieval quality has remained stable over the years inspected, 2006 through 2011.

Nadir Water Vapor

TES Version 6 H_2O is typically biased high relative to Version 5 H_2O. The changes are largely due to much higher H_2O mixing ratios in the *a priori* constraint, GMAO GEOS 5.9.1 (in Version 6) versus GEOS 5.2 (in Version 5). The largest effect is seen at low degrees of freedom for signal (DOFS). The user should select data using the master data quality flag ("speciesretrievalquality") and filter by DOFS. Some minor changes are due to new ABSCO tables for H_2O, a few percent difference at most.

TES uses an optimal estimation non-linear least squares retrieval (Bowman et al., 2006). TES Versions 5 and 6 use a wide band retrieval (1100 to 1330 cm^{-1}) to jointly estimate the mixing ratios of four species: HDO, H_2O, CH_4, and N_2O (Worden et al., 2012). This retrieval dramatically improves the vertical resolution in the lower troposphere for water vapor, compared to Version 4. Comparisons have been made between TES Version 5 water vapor profiles and radiosonde profiles, demonstrating greater sensitivity to boundary layer water vapor than previous versions. Relative to the NOAA ESRL global radiosonde database, TES Version 5 water vapor has a small bias of +10% to -12% in the lower troposphere, with a positive bias up to +15% in the middle troposphere at 400 hPa. The rms differences tend to increase from 30% near the surface to 50% in the middle troposphere.

Nadir HDO

TES Version 6 estimates of HDO/H_2O have been compared to Version 5, as shown in Figure 1. Differences are mostly uniform across all latitudes. In the free troposphere, Version 6 is biased slightly lower than Version 5 by -1.1 per mil. In the boundary layer, however, Version 6 is biased *higher* than Version 5 by approximately +6 per mil.

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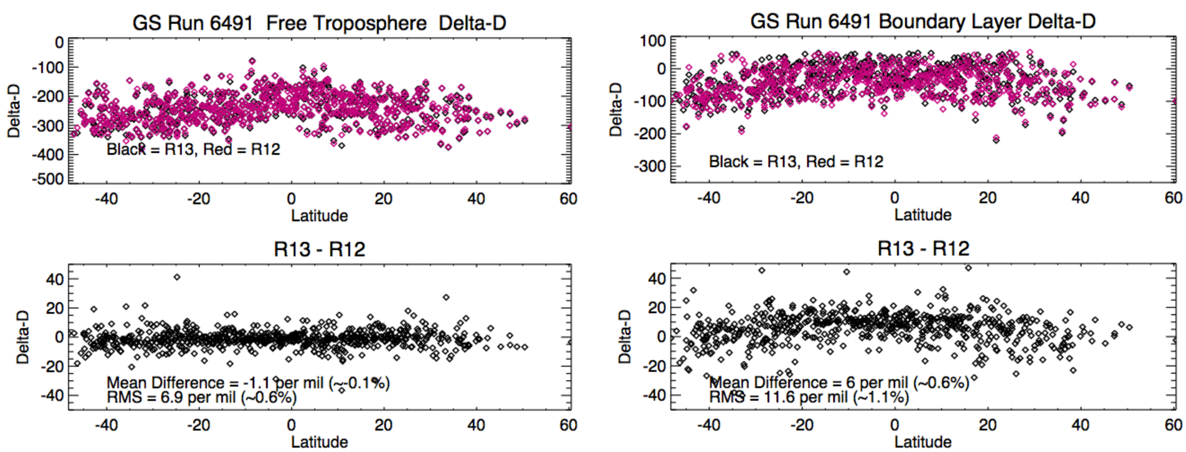

Figure 1: comparisons of TES Version 6 ("R13") and Version 5 ("R12") delta-D isotopic signature of HDO/H_2O from Global Survey 6491.

Version 5 and Version 6 estimates of HDO/H_2O show considerable sensitivity to the isotopic composition of water vapor with typically DOFS~2 in the tropics and DOFS~1 at high latitudes. This increased sensitivity allows the TES estimates to resolve lower tropospheric and mid-tropospheric variability of the HDO/H_2O vapor ratio (see Worden et al., 2012) with the expense of increased uncertainty over tropical oceans.

We find that the HDO/H_2O estimates are consistent with the previous TES release within the altitude range where the sensitivity overlaps. However, Version 5 is biased higher than Version 4 by approximately 7.5 per mil. Consequently, the estimated bias correction factor for Version 5 should be 5.55% (J. Worden et al., 2011).

For validation of Version 4 HDO/H_2O, we refer the reader to J. Worden et al. (2011).

Nadir Ammonia (NH_3)

Ammonia (NH_3) is a standard product in TES Version 6. The Version 6 algorithm update had little impact on the retrieved profiles. Occasionally Version 5 and Version 6 selected different a priori profiles (see example in upper right column), which led to different retrieved profiles shapes, but similar "representative tropospheric volume mixing ratio" (RTVMR), as to be expected in these cases with high degrees of freedom for signal (DOFS). In general, TES can detect spatial variability and seasonal trends in NH_3. The TES NH_3 signals appear well correlated with *in situ* measurements when averaged over time and/or space over regions with not ideal observing conditions, such as eastern China or North Carolina.

Two validation cases show ideal retrieval conditions of high NH_3 concentrations, elevated temperatures and few clouds in the San Joaquin Valley of California during Discover-AQ (January 2013). In these cases, it is possible to compare non-averaged TES signals with *in situ* measurements and show that both present similar spatial variability. First, Versions 5 and 6 TES RTVMR NH_3 were compared with airborne Picarro and PTR *in situ* measurements. All four datasets are very well correlated, especially TES Version 6 and the PTR data. Differences in magnitude arises from the difference in sensitivity: the aircraft measurements are taken at approximately 500 m AGL, while TES is most sensitive, in this region, between 1 and 2 km AGL; at these altitudes the NH_3 concentration is usually well correlated with the values at lower

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levels, but the ratio between the NH_3 concentrations is dependent on the structure of the boundary layer. Note however that even the two aircraft instruments flying on the same plane show notable differences between 35.8 N and 36.2 N, illustrating the difficulty of obtaining accurate NH_3 measurements.

Second, TES Version 6 RTVMR NH_3 was compared to *in situ* measurements from the Open Air QCL instrument mounted on an automobile following the TES geolocation track. As in the aircraft comparisons, the TES and ground measurements are well correlated, but have different numerical values.

Formic Acid (HCOOH)

TES retrieves a "representative tropospheric volume mixing ratio" (RTVMR) of formic acid (HCOOH). Preliminary data analysis shows 90% good data throughput. Of these good cases, 80% have DOFS > 0.1. We are awaiting processing of GMAO GEOS 5.9.1 temperature and water vapor in order to process the TES retrievals for key validation dates.

Methanol (CH_3OH)

Similar to formic acid, TES retrieves a methanol RTVMR. We are awaiting processing of GMAO GEOS 5.9.1 temperature and water vapor in order to process the TES retrievals for key validation dates.

Nadir Methane

The validation of the TES CH_4 product is sufficient to characterize the latitudinal dependence of the mean bias and the instrument error. Work so far suggests that TES CH_4 contains useful information when viewed using the "representative tropospheric volume mixing ratio" (RTVMR) approach. In order to assess the data quality of the Version 6 CH_4 product, we have initially compared Version 6 results to Version 5 results for a global survey taken during the timeframe of the HIPPO I aircraft campaign. For CH_4, Version 5 data quality had previously been assessed by comparison to in-situ aircraft profile measurements from the HIPPO I and II aircraft campaigns. The Version 5 data had been found to broadly capture the latitudinal gradient in CH_4 as observed by HIPPO measurements. Version 5 representative tropospheric mixing ratios (RTVMRs) were biased high by around 40 ppbv compared to HIPPO values. We find that for global survey observations, the throughput for Version 6 is very similar to the throughput for Version 5. Version 6 values are reduced by ~10 ppbv compared to Version 5. We can infer that this will result in a smaller bias relative to the HIPPO measurements.

Changes between Version 6 and Version 5 that could affect the CH_4 result include updates to spectroscopy and updates to various datasets used as initial guess and *a priori* information. Version 6 includes spectroscopy updates for CO_2, H_2O and CH_4. Of these, the CH_4 spectroscopy update is the only one expected to have an appreciable effect on the CH_4 retrievals. Version 6 also includes updated GMAO v5.9.1 fields (TES CH_4 retrievals are somewhat sensitive to changes in temperature and H_2O), as well as updates to the CH_4 and N_2O climatologies used as

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initial guess and *a priori* information. Latitudinal differences between Version 6 and Version 5 CH_4 are understood to be largely due to the N_2O climatology (specifically the tropopause height and corresponding N_2O dropoff in the stratosphere).

Figure 2 shows Version 6 and Version 5 CH_4 values, and the differences between versions for an example global survey (runid 10218) during the HIPPO I campaign.

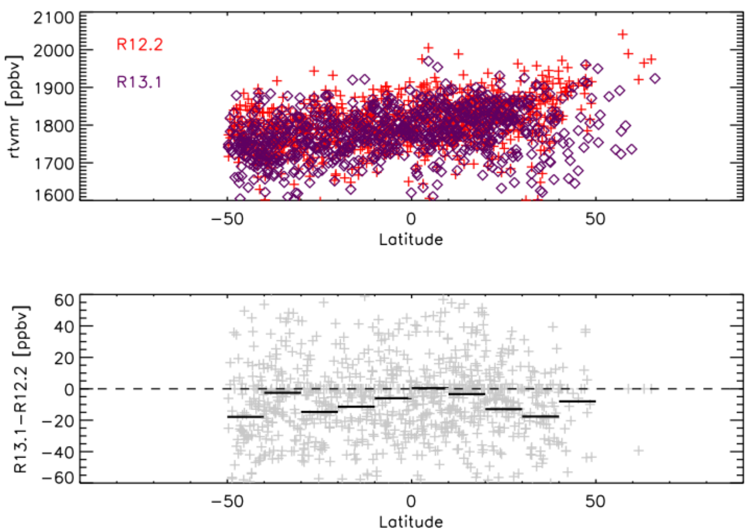

Figure 2: Upper panel shows Version 5 and Version 6 representative tropospheric volume mixing ratios (RTVMRs) for a single global survey (runid 10218), for cases where the degrees of freedom for signal is greater than 1.6. Lower panel shows the differences between Version 6 and Version 5. Black horizontal bars show mean differences within 10 degree latitude bins.

Nadir Surface Temperature (Sea Surface Temperature)

TES retrieves surface (skin) temperature as standard product. Over ocean this amounts to a sea surface temperature (SST). TES retrievals of SST rely on validation of V003. 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.

TES Nadir Cloud Products

Version 5 TES cloud products have been 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

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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 products

Limb products have not changed from V004, see the V004 quality statement for descriptions for these.

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