Aura-TES L2 Products: Version 5 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, 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 the latest version of TES data (V005, F06_08 and F06_09) are available in an updated TES Validation Report (Herman et al., 2012), including V005 L1B radiances. The subsections below give an overview of the validation and data quality analysis of TES V005 data and/or on the quality of earlier versions of the TES data products.

There have been thirteen papers published in a special issue of Journal of Geophysical Research Atmospheres dealing with Aura validation published in 2008. These, plus additional validation papers and other TES publications, are available at the TES publications web site.

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 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).

In April 2010, TES implemented a new strategy for observing and processing calibration measurements (see Section 4 for details). 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 V005 ozone profiles is nearly identical to that of TES V004. The changes in retrieval algorithm for other trace gases in the TES V005 products are not expected to downgrade the quality of ozone profiles. The TES V004 validation report, a version prior to this one, showed that the percent and absolute biases of TES-sonde are congruent to previous validation studies of TES V001 and V002. Hence, verifying the consistency between the percent and absolute biases of TES V005 and that of TES V004 is sufficient to validate TES V005 nadir ozone profile. TES V005 nadir ozone profiles provide data that were measured in the TES global survey, step-and-stare, transect, and stare observation modes. They were compared with ozonesonde measurements from multiple datasets that have been used in the TES V004 validation. The percent and absolute differences between TES and ozonesonde were investigated in six latitude zones. The seasonal variability of ozone was investigated by using the 904 TES-sonde coincidences in the 35° N to 56° N latitude zone.

The criteria of ±9 h, a 300 km radius and a cloud optical depth less than 2.0 were applied to search for the TES-sonde coincidence measurements. The flagged TES data were filtered out. 1907 matches were found from those TES measurements that have been processed for V005. Their latitude range is from 72.5° S to 81.8° N and time spans from 2006 to 2010. The TES averaging kernel and a priori constraint were applied to the ozonesonde data in order to: 1) compare the TES ozone profiles and ozonesonde data in an unbiased quantifiable manner (i.e. not biased by the TES a priori) 2) take TES measurement sensitivity and vertical resolution into account.

In general, TES V005 ozone profiles are positively biased (by less than 15%) from the surface to the upper-troposphere (~ 1000 to 100 hPa) and negatively biased (by less than 20%) from the upper-troposphere to the lower-stratosphere (100 to 30 hPa) when compared to the ozone-sonde data. Both V004 and V005 TES data showed the mean bias is from -14 to +15% and the one standard deviation is from 5 to 20%. The absolute mean percent differences for all seasons for mid-to-lower tropospheric ozone also show an improvement when compared to Nassar et al. (2008). All of these features are consistent with that of Boxe et al. (2010) and TES V004 validation report (Herman et al., 2011).

Nadir Carbon Monoxide

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 40S and 45N, 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 650 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 V005 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 over land at the SGP Arm site (Riley et al., 2009). Further details of this validation can be found in Kulawik et al. (2012). This validation was done with the prototype code which is nearly identical to the production code (PGE), but has some minor differences due to differences in the altitude grid calculation. The HIPPO analysis can be done with the processed PGE (Product Generation Executive) data, but the SGP analysis requires a full time series of TES at the SGP site and will need to await a more complete V005 dataset. Analysis of the PGE comparisons to HIPPO show about a 1.2 ppm error and an overall -0.7 ppm bias, as compared to the prototype which has about a 1.1 ppm error and an overall bias of +0.5 ppm. There are some outliers in the monthly mean values from both the prototype and the PGE and we are working on additional quality flags to screen these out. A fuller set of TES data needs to be examined before the V005 bias is officially set as different sites and times have relative biases on the order of 0.5 ppm. The single target error for TES CO_2 in the mid-Troposphere is on the order of 8 ppm, however averaging over 20 degrees longitude, 10 degrees latitude, and 1 month results in errors on the order of 1 ppm over both ocean and land targets. Through comparisons to validation data, we have found that the errors are underpredicted by a factor of about 1.5, and that the averaging kernel needs be corrected to account for the TES multi-step retrieval. The details of this correction are found in Kulawik et al. (2012) which involves a pressure-dependent scale factor. Although the TES CO_2 product is modest both in sensitivity and coverage, Nassar et al. (2011) found that TES added information to the surface flask measurements and was useful for estimating fluxes, both separately, and jointly with flask measurements. We have also recently found (manuscript in preparation) that TES assimilation into GEOS-Chem improves the amplitude of the mid-tropospheric CO_2 seasonal cycle as compared with aircraft profiles measured at the SGP-Arm site.

Nadir Atmospheric Temperature

TES V005 nadir temperature (TATM) retrievals have been compared with nearly coincident radiosonde (hereafter sonde) measurements from the NOAA ESRL global sonde database. For TES V005 TATM minus Tradiosonde (with averaging kernel applied), the bias is +0.2 to +0.5 K in the lower troposphere, -0.5 K in the upper troposphere. This is an improvement over previous versions of TES TATM. The rms is less than 1 K in the stratosphere and upper troposphere, but increases to 1.7 K in the lower troposphere. In clear sky conditions (average cloud effective optical depth less than 0.1), the bias improves in the lower troposphere but increases to +0.5 K at 500 hPa pressure level.

To evaluate the retrieval stability the monthly mean and standard deviation of the TATM residual between TES 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 from 2006 - 2011.

Nadir Water Vapor

TES uses an optimal estimation non-linear least squares retrieval (Bowman et al., 2006). The latest version V005 uses 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 new retrieval dramatically improves the vertical resolution in the lower troposphere for water vapor. Comparisons have been made between TES V005 water vapor profiles and radiosonde profiles, demonstrating greater sensitivity to boundary layer water vapor than previous versions. Comparisons were also made with the NOAA ESRL global radiosonde database for close coincidences of <100 km and -0.5 hours to +1.5 hours. TES V005 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

For validation of V4 HDO, we refer the reader to Worden et al. (2011).

V5.1 estimates of HDO/H_2O show considerable more sensitivity to the isotopic composition of water vapor with typically 2 DOFS of freedom in the tropics and ~1 DOF 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, the new version is biased higher by approximately 7.5 per mil. Consequently, the estimated bias correction factor for V5.1 should be 5.55% (Worden et al., 2011).

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. TES shows a positive mean bias of 1.0% - 3.7% with random instrument error of 1.4% - 1.6% with respect to measurements made during the first two HIPPO missions. TES successfully captures the latitudinal gradient observed during HIPPO I and II.

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

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.

Ammonia

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. When there are high concentrations, warm temperatures and few clouds, as in the San Joaquin Valley, it is possible to compare non-averaged TES signals with in situ measurements and show that both present similar spatial variability.

Limb Products

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

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