Aura-TES L2 Products: Version 8 Data Quality Description

Overview of Current Data Quality Status

This is a report on data quality of TES Version 8 data (V008, files ending in F08_12). There is one new standard TES product in V008, the chemical species hydrogen cyanide (HCN). V008 continues the same standard TES products as V007, including TES L1B radiances, ozone, carbon monoxide, atmospheric temperature, water vapor, HDO, methane, sea surface temperature, cloud properties, carbon dioxide, formic acid (HCOOH), methanol (CH_3OH), ammonia, peroxyacetyl nitrate (PAN), carbonyl sulfide (OCS) and the Instantaneous Radiative Kernel (IRK). Level 2 data nadir products are all validated and usable in scientific analyses. Details on the validation of TES standard products are available in the TES V008 Data Validation Report (Herman et al., 2019).

The subsections below give a brief overview of the latest data quality analysis of TES V008 and/or V007 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 and Kulawik, 2020) 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 documents web site.

Users should also read the data 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 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.

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

New Product Hydrogen Cyanide (HCN)

Hydrogen cyanide (HCN) is a new product in TES V008. TES is sensitive to HCN in the upper troposphere (e.g. 200 hPa) and therefore will primarily observe fire signatures with high injection heights. TES HCN is the first product to be retrieved in linear volume mixing ratio (VMR). This has the advantage of resulting in very consistent sensitivity over the large range of retrieved HCN, but also may result in negative HCN values. The initial guess and a priori for HCN are set to a constant value of 100 parts per trillion by volume (pptv).

Validation of HCN is from the global distribution of HCN for October, 2006. The large Indonesian fires of that month have a verified large HCN signal in the TES V008 data.

Nadir Ozone

The retrieval algorithm for TES V008 is largely the same as that for the V007 data set. There were few changes in the retrieval code for this latest version of the TES that affect the ozone retrievals and the comparisons to ozonesondes support that conclusion. The changes to the retrieval system are mostly in the Level 1B steps, including updates to radiance spike detection and path difference thresholds. Previous versions of the TES Validation Report have shown the consistency in the ozone retrievals as the retrieval system has evolved.

TES V007 nadir ozone profiles have been compared with ozonesonde measurements archived in the World Ozone and Ultraviolet Radiation Data Center (The Global Atmosphere Watch Programme (GAW) of the World Meteorological Organization (WMO), 2017). As of the writing of this document, the TES ozone retrievals have been matched with ozonesonde data with coincidence criteria of ±9 hours and 300 km distance and a limit on the cloud optical depth of a value less than 2.0. The comparison of the differences between the V008 ozone retrievals with the sondes and corresponding V007 data show very consistent results. Looking at the mean values for 2005-2010, the V008 data agreed slightly better with the sondes in the troposphere by about 4-6 percent. The bias and error statistics generally show an improvement when compared to earlier ozonesonde comparisons published by Nassar et al. (2008) and Boxe et al. (2010).

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 (Measurement Of Pollution In The Tropopsphere) 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.

Nadir Atmospheric Temperature

TES V008 nadir temperature (TATM) retrievals have been compared with nearly coincident radiosonde measurements from the National Oceanic and Atmospheric Administration (NOAA) Earth Science Research Laboratory (ESRL) global radiosonde database. Generally, V008 TATM is very similar to the previous V007 data.

To evaluate the retrieval stability the monthly mean and standard deviation of the TATM residual between TES V005 and the Global Modeling and Data Assimilation Office (GMAO) GEOS-5.2 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 a five-and-a-half year period of 2006 through 2011. The standard deviation of the residual was generally smaller than the standard deviation of the GMAO GEOS-5.2 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 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.

Nadir Water Vapor

TES V008 H_2O has been compared to V007 H_2O. On average, the mean differences between V008 and V007 are insignificant. The user should select data using the master data quality flag ("speciesretrievalquality") and filter by degree of freedom for signal (DOFS).

Nadir HDO/H_2O

TES V008 estimates of HDO/H_2O have been compared to V007. There is essentially a zero-mean difference between the versions and the uncertainty calculation between versions are consistent. V008 HDO/H_2O shows considerable sensitivity to the isotopic composition of water vapor with typical degrees of freedom for signal (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.

Nadir Methane

Here, we reference the V008 methane results to the V006 results that were validated against the HIAPER Pole-to-Pole Observations (HIPPO) campaign (Alvarado et al., 2015). Using 37 TES global surveys from the time periods of the HIPPO campaign, we find that the mean difference between V006 and V007 is less than 4 parts per billion by volume (ppbv) at all altitudes for both uncorrected and N_2O-corrected profiles, with standard deviation less than 37 ppbv at all altitudes. Therefore, the biases between V008 and V006 are relatively small compared to the biases with respect to the HIPPO aircraft profiles.

Nadir Carbon Dioxide

TES CO_2 is retrieved between 40°S and 45°N, with average cloud effective optical depth < 0.5, among other tests, for good quality. Errors tend to be correlated for close locations and times, and it is recommended to use TES data averaged in 10° by 10° by 1 month averages, both to mitigate correlated errors and reduce errors to useful levels. On average, TES CO_2 has an average of 0.65 degrees 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 hPa, with the most sensitivity between about 700 and 300 hPa, peaking at about 650 hPa. Although a profile is retrieved, there is very little independent information at the different profile levels and it is necessary to utilize the provided averaging kernel when using TES data. Most of the validation has been performed at the 510 hPa pressure level. TES V008 CO_2 is compared with aircraft vertical profiles over the Pacific from the High-Performance Instrumented Airborne Platform for Environmental Research (HIAPER) Pole-to-Pole Observation (HIPPO) program (Wofsy, 2011). The error assessment follows Kulawik et al. (2019), which estimates systematic and random errors, such that the error for an average of n observations equals sqrt(systematic^2 + random^2/n). The TES observations have an overall bias of -1.1 parts per million by volume (ppmv) versus HIPPO, a systematic error of 1.4 ppmv, and random error of 7.3 ppmv. This is similar to the previous V007 errors, which were estimated to be a random error of 6 ppmv, and a correlated error of 1.7 ppmv.

Level 2 Instantaneous Radiative Kernel (IRK)

Level 2 TES Instantaneous Radiative Kernel (IRK) just for ozone over 9.6-micron ozone band was a standard product in TES V006 using a 3-point Gaussian integration method. In TES V007 and V008, we use a 5-point Gaussian integration, a computationally more expensive but more accurate method, to compute IRK and expand the IRK products to include 1) 9.6-micron band TOA flux (980 – 1020.2 cm^{-1}), 2) both IRK and LIRK (logarithm IRK) for O_3 and water vapor (H_2O), 3) LIRK for cloud optical depth (COD), cloud top pressure (CTP), and emissivity (EMIS), and 4) IRK for atmospheric temperature (TATM) and surface temperature (TSUR). These products have been validated individually with prototype (IDL) code calculations (Kuai et al., 2017) using one global survey observations.

The statistics (the mean and one standard deviation) for the fractional differences between Product Generation Executive (PGE) and prototype of all IRK products' calculated using the same Jacobians for integration are showed to have negligible differences (1E-06% ± 3E-06%). The global pattern for all products are well replicated by PGE algorithm.

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 Atmospheric Infrared Sounder (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.

TES Nadir Cloud Products

TES retrievals of cloud products rely on validation of previous data versions, as described in detail in the TES Validation Report V005 (Herman et al., 2012). Here is a brief summary. V005 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 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.

Nadir Ammonia (NH_3)

Ammonia (NH_3) is a standard product in TES V008. The V008 algorithm update had little impact on the retrieved profiles, with insignificant bias between versions V008 and V006. TES NH_3 provides useful information over regions with moderate to strong NH_3 sources. Due to the sparse TES coverage and the weak signal from NH_3, single TES observations have large uncertainties, except over regions with very high NH_3 concentrations. However, spatial and temporal averages show good correlation with chemical transport model (CTM) output and with in situ measurements.

Formic Acid (HCOOH)

TES V008 formic acid (HCOOH) provides useful information over regions with strong HCOOH sources, e.g. biomass burning events. Due to the sparse TES coverage and the weak signal from HCOOH, single TES observations have large uncertainties. However, spatial and temporal averages show good correlation with CTM output and with the very limited set of co-located in situ measurements.

Methanol (CH_3OH)

TES methanol (CH_3OH) has a weak signal and an a priori distribution chosen as a function of location and date. The information content of the retrieval is quite low, but seasonal averages over large regions do provide useful information for evaluating CTMs.

Nadir Peroxyacetyl Nitrate (PAN)

Peroxyacetyl nitrate (PAN) V007 retrievals (as well as prototype results that preceded V007) have been extensively utilized in peer-reviewed publications. Therefore, we have performed a preliminary assessment of the V008 PAN product by (1) comparing to TES observations/time periods that have previously been utilized in publications and (2) verifyinng consistency between V007 and V008.

Payne et al. (2014) showed examples of elevated CO and PAN in boreal burning plumes (previously identified by Alvarado et al., 2010) seen in TES special observations made during the July 2008 phase of the ARCTAS campaign. These plume examples showed strong evidence for PAN enhancements in fire plumes and demonstrated that it was possible for adjacent TES pixels to show sharply different PAN volume mixing ratios. Although coincident aircraft data were not available, the retrieved PAN values, between zero and 1.5 ppbv, were deemed to be reasonable, given the range of PAN values measured from aircraft during the campaign (Alvarado et al., 2010; Roberts et al., 2009). Payne et al. (2017) showed prototype PAN retrieval results for the Tropics in austral spring, showing a maximum in PAN over the tropical Atlantic, a feature that had been predicted by models and also previously observed using limb-sounding satellite measurements.

The PAN algorithm has not changed between V007 and V008, but there have been updates to the spectroscopy of interfering species that could cause minor changes to the retrieved PAN. Payne et al. (2014) showed that the dominant sources of error in the TES PAN retrievals are instrument noise, water vapor and ozone. V007 uses the ABSCO v2.5 tables, while V008 uses ABSCO v3.0.

Nadir Carbonyl Sulfide (OCS)

The data quality of the TES V008 Carbonyl Sulfide (OCS) product has been assessed through comparisons between TES OCS and aircraft measurements collected during five HIAPER Pole-to-Pole (HIPPO) campaigns during months of January, March to April, June to July, August to September, and November.

The latitudinal distribution in TES OCS is consistently varying with HIPPO observations with root-mean-square of the differences for individual comparison range from 3 to 7 pptv. The global bias is approximately 1.46 pptv with an error standard deviation of about 5.97 pptv. The correlation coefficients between TES OCS and HIPPO for five campaigns are on average of 0.8.

Limb products

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

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