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Earth Observing System (EOS)
Tropospheric Emission Spectrometer (TES)

Level 2 (L2) Data User's Guide
(Up to & including Version F04_04 data)

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1.0	4/12/2006	Initial Version of TES L2 Data User's Guide
2.0	6/1/2006	TES L2 Data User's Guide (Up to & Including F03_03 Data)
3.0	5/4/2007	TES L2 Data User's Guide (Up to & Including F04_04 Data)
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1. Scope of this Document

This document will provide an overview of the TES instrument and the Level 2 (L2) volume mixing ratio (vmr) and temperature profile data that it measures. The document should provide an investigator the information necessary to successfully use TES data for scientific studies.

This document discusses TES L2 data version F04_04 as well as prior versions.

This document should be considered an overview of the TES instrument and data, but many additional sources of information are available. The primary sources of information about TES data and data product files are:

- *TES Data Products Specification (DPS) Documents* (Lewicki, 2005a; Lewicki, 2005b; Lewicki, 2005c; Lewicki, 2007) - The DPS documents provide extensive information about the data product file content, file sizes and obtaining TES data.
- *TES L2 Algorithm Theoretical Basis Document* (Osterman et al., 2004) - This document provides information about the TES L2 retrieval algorithm, support products and forward model.
- *TES Validation Report* (Osterman et al., 2007a) - TES data products are currently undergoing an extensive validation of their scientific quality. An overview of initial validation results is provided in Section 8. More information about validation of the TES L2 products can be found in the TES Validation Report.

There are several other documents that provide important information about TES and they are listed according to subject in the references Section 9.

Users of TES data are encouraged to contact the TES science team for further guidance on successfully applying and interpreting the data products. Contact information for TES team members is available at the TES web page (http://tes.jpl.nasa.gov/team/index.cfm).

2. An overview of the TES instrument

2.1 Instrument Description

The Tropospheric Emission Spectrometer (TES) on EOS-Aura was designed to measure the global, vertical distribution of tropospheric ozone and ozone precursors such as carbon monoxide (Beer et al., 2001; Beer, 2006). TES is a nadir and limb viewing infrared Fourier transform spectrometer (FTS) (http://tes.jpl.nasa.gov/mission/instrument.cfm). The TES spectral range is from 650 to 3250 cm^{-1}. The apodized resolution for standard TES spectra is 0.10 cm-1, however, finer resolution (0.025 cm^{-1}) is available for special observations. The footprint of each nadir observation is 5 km by 8 km, averaged over detectors. Limb observations (each detector) have a projection around 2.3 km x 23 km (vertical x horizontal).

TES is on the EOS-Aura platform (http://aura.gsfc.nasa.gov/) in a near-polar, sun-synchronous, 705 km altitude orbit. The ascending node equator crossings are near 1:45 pm local solar time.

2.2 TES Observation Modes

2.2.1 Global Surveys

TES makes routine observations in a mode referred to as the "global survey". A global survey is run every other day on a predefined schedule and collects 16 orbits (~26 hours) of continuous data. Each orbit consists of a series of repetitive units referred to as a sequence. A sequence is further broken down into scans. Global surveys are always started at the minimum latitude of an Aura orbit. Table 2-1 provides a summary of the initial and modified versions of the TES Global Surveys from Launch to the present day.

Table 2-1 Description of TES Global Survey Modifications

Start Date/ First Run ID	Scans	Sequences	Maximum Number of TES L2 Profiles	Along-Track Distance between Successive Nadir Scan Locations	Description
August 22, 2004 / First GS Run ID 2026 (First 4 GS runs were 4 orbits only) (First full GS is Run ID 2147/Sep 20, 2004)	3 Limb/ 2 Nadir	1152 sequences (72 per orbit)	Maximum of 4608 L2 profiles (1152 sequences x (3 Limb Scans+ 1 Nadir Scan))	~544 km	• At-launch Global Survey (Aura launched on July 15, 2004) • Each sequence composed of 2 calibration scans, 2 nadir viewing scans and 3 limb scans. • The two nadir scans were acquired at the same location on the spacecraft ground track. Their radiances were averaged, providing a single TES L2 profile.

Start Date/ First Run ID	Scans	Sequences	Maximum Number of TES L2 Profiles	Along-Track Distance between Successive Nadir Scan Locations	Description
May 21, 2005 / Run ID 2931	3 Nadir	1152 sequences (72 per orbit)	Maximum of 3456 L2 profiles (1152 sequences x 3 nadir scans)	~182 km	• Global survey was modified to conserve instrument life. • Three limb scans were eliminated and replaced by an additional nadir scan. • The 3 Nadir scans were acquired at locations equally spaced along the spacecraft ground track. The radiances of individual scans are not averaged.
January 10, 2006 / Run ID 3239.	3 Nadir	1136 sequences (71 per orbit)	Maximum of 3408 L2 profiles (1136 sequences x 3 nadir scans)	~182 km	• The last sequence in each orbit was replaced with an instrument maintenance operation.
June 6, 2008 / Run ID 7370.	3 Nadir	960 sequences (60 per orbit)	Maximum of 2880 L2 profiles (960 sequences x 3 nadir scans)	~182 km	• Global survey was modified to conserve instrument life. • No measurements poleward of 60°S latitude.
July 30, 2008 / Run ID 8187.	3 Nadir	768 sequences (48 per orbit)	Maximum of 2304 L2 profiles (768 sequences x 3 nadir scans)	~182 km	• Global survey was further modified to conserve instrument life. • No measurements poleward of 50°S, 70°N latitude.

2.2.2 Special Observations

Observations are sometimes scheduled on non-global survey days. In general these are measurements made for validation purposes or with highly focused science objectives. These non-global survey measurements are referred to as "special observations". Eight special observation scenarios have been used to date and are summarized in Table 2-2.

Table 2-2 Description of TES Special Observation Modes

Name	Dates	Pointing	Sequences	Scans per Sequence	Distance Between Scans	Comments
Step and Stare	Sep 2004 through Aug 6, 2005	Nadir	6	25	40 km	Continuous along-track nadir views, ~45 degrees of latitude.

Name	Dates	Pointing	Sequences	Scans per Sequence	Distance Between Scans	Comments
Step and Stare	July 1, 2007 through present	Nadir	1	165	40 km	Along track nadir observations spanning 65 degrees of latitude
Step and Stare	Jan 17, 2006 – Oct 8, 2006 and 2008	Nadir	1	125	45 km	Continuous along-track nadir views, ~50 degrees of latitude.
Note: In 2008 both the 125 and 165 scan Step and Stare macros were used						
Transect	Jan 16, 2006 through present	Near Nadir	1	40	12 km	Hi density along-track or off nadir views.
Transect	Aug 20, 2005 – Sept 2, 2005	Near Nadir	1	68	25 km	Hi density along-track or off nadir views.
Stare	Launch through present	Near Nadir	1	32	0 km	All measurements at a single location.
Limb Only	Jan 31, 2006 – May 20, 2006	Limb	1	62	45 km	Continuous along-track limb views, 25 degrees of latitude.
Limb HIRDLS	Feb 13, 2006 Only	Limb	142	3	182 km	2 orbits of continuous limb measurements for HIRDLS (High Resolution Dynamics Limb Sounder) comparison

2.3 TES Scan Identification Nomenclature

Each TES scan is uniquely identified by a set of three numbers called the run ID, the sequence ID and the scan ID. Each major unit of observation is assigned a unique run ID. Run IDs increase sequentially with time. The first on-orbit run ID is 2000. The sequence ID is assigned to repetitive units of measurements within a run. They start at 1 and are automatically incremented serially by the TES flight software. The scan ID is also incremented by the flight software each time a scan is performed. Each time the sequence is set to 1, the scan ID is reset to 0.

Each time TES makes a set of measurements, that data set is assigned an identification number (referred to as a "run ID"). A calendar of the TES run IDs for global surveys and a list of all TES run IDs (including observation data, time and date) can be found at http://tes.jpl.nasa.gov/science/dataCalendar.cfm .

3. Where to Obtain TES Data

There are two locations for obtaining TES data. Links to both locations are available from the TES site at the Langley Atmospheric Science Data Center (ASDC) http://eosweb.larc.nasa.gov/. The supporting documentation necessary to use TES data is also available at the Langley ASDC site.

- The primary location for obtaining TES data is the Earth Observing System (EOS) Data Gateway (http://redhook.gsfc.nasa.gov/~imswww/pub/imswelcome/).
- The second location for obtaining TES data is the Langley ASDC data pool. The data pool has space limitations that make it somewhat dynamic, therefore older versions of TES data may not be available there.

The TES data files are listed in different ways for the different sites. The naming convention will be described in Section 4.1.

All TES data products are in HDF-EOS 5 format and are completely documented in the TES Data Product Specification documents referenced in Section 9. The site also contains links to the TES documentation mentioned in this manuscript.

4. An Overview of TES L2 Data Products

4.1 File Formats and Data Versions

Information about the TES data file content and format versioning can be found in the L2 product filenames. Table 4-1 provides information for differentiating between the TES versions. When ordering the data on the EOS Data Gateway, the TES level 2 products can be initially differentiated by the TES Product (ESDT or Earth Science Data Type) version label shown in the first column of Table 4-1. Once the data is downloaded, more information can be gathered from the TES version string in the filename.

The TES L2 Data Products are provided in files separated out by the atmospheric species being measured. The parts of the product filename are:

<inst.>-<platform>_<process level>-<species>-<TES view mode>_r<run id>_<version id>.he5

The TES Version String (version id), contains the Format and content version:

F<format version>_<science content version>

A change to the format version string corresponds to minor updates to the fields available within the file or minor bug fixes. Changes to the science content string reflect major changes in the science content of certain fields in the data products.

An example file name is:

TES-Aura_L2-O3-Nadir_r000002945_F04_04.he5

This particular file contains TES nadir measurements of ozone for run ID 2945 (000002945).

In addition to the atmospheric products, there are data files with additional (ancillary) data that are important for working with TES data. These ancillary files can be used with any species data file and contain the string "Anc" in the filename.

Table 4-1 provides a way to map the TES version string information to the TES data product version. For example, version F03_03 is the first version to contain limb data and version F03_02 data was a significant upgrade to the science content in the data products and therefore is referred to as version 2 (V002) TES data. When ordering TES Level 2 data products through the EOS Data Gateway, the products will be grouped by the TES version number (ESDT) in a form that looks like:

TES/AURA L2 O3 NADIR V003.

If the TES data is ordered through the Langley ASDC Data Pool using the FTP (File Transfer Protocol) interface, the version 3 nadir ozone data will be listed in the form:

TL2O3N.003.

If the TES data is ordered through the Langley Data Pool using the Web interface, the version 3 nadir ozone data will be listed as:

TL2O3N.3.

While the data may be listed differently for the different sites for downloading the products, the filenames will be identical.

There are currently five different versions of TES L2 data products. It is currently planned that all TES L2 data products should be processed with the latest software release by late December 2007 (complete set of V003 (F04_04) L2 data products). Until this time, there will be a mixture of F03_03 and F04_04 data products available. Data from versions prior to V002 (F03_03) are no longer publicly available, but the evolution of the product versions and file formats is provided back to V001 (F01_01 and F02_01).

Table 4-1 Description of the TES L2 Data Product Version Labels

TES Product (ESDT) Version	TES Version String	Format Version	Science Content Version	Description
V001	F01_01	1	1	The first publicly released L2 data
V001	F02_01	2	1	Bug fixes and additional fields
V002	F03_02	3	2	Some additional fields but major upgrade to scientific quality of data.
V002	F03_03	3	3	Limb data and some bug fixes
V003	F04_04	4	4	Improvements to nadir ozone, temperature, methane and to limb products. Fully processed from Sep 2004 through present.

4.2 TES Standard L2 Products

Currently the TES data products available for any given run ID are listed in Table 4-2. The products are separated by species with an ancillary file providing additional data fields applicable to all species. A description of the contents of the product files, information on the Earth Science Data Type names and file organization can be found in the TES DPS documents (Lewicki, 2005a; Lewicki, 2005b; Lewicki, 2005c; Lewicki, 2007).

Table 4-2 Description of the TES L2 Data Product Files Currently Available

TES L2 Standard Data Product	TES View Mode	Description
Ozone	Nadir and Limb	TES ozone profiles and some geolocation information
Temperature	Nadir and Limb	TES atmospheric temperature profiles and some geolocation information.
Water Vapor	Nadir and Limb	TES nadir water vapor profiles and some geolocation information

TES L2 Standard Data Product	TES View Mode	Description
Carbon Monoxide	Nadir	TES nadir carbon monoxide profiles and some geolocation information
HDO	Nadir and Limb	TES HDO profiles and some geolocation information
Methane	Nadir	TES nadir methane profiles and some geolocation information
Nitric Acid	Limb	TES limb nitric acid profiles and some geolocation information
Ancillary	Nadir and Limb	Additional data fields necessary for using retrieved profiles.

TES retrieves surface temperature and it is reported in each nadir species file, however the value in the atmospheric temperature file is the one that should be used for scientific analysis.

4.3 TES Version F04_04 Data

This is the most current version of the TES L2 data products. The limb products are improved but should still be used with caution, particularly in the troposphere. The methane product (nadir) is also improved, but is still being refined. This version of the TES L2 data was created using the "Release 10.x" or "R10.x" software and any reference to R10 TES data are consistent with the F04_04 label. It is also referred to as TES version 3 (V003) data.

4.3.1 Known Issues or Advisories for the TES Version F04_04 Data

The TES team has determined a few instances where the most recent data product version should not be used for scientific analysis or used with caution. These are listed below and should be fixed in a future version of the TES data. Also included below are warnings about certain data fields.

- In this version the nadir L2 profiles are reported on a 67 level grid.
- Data is not reported for failed target scenes. Consequently, file sizes will differ between runs.
- Fill value for data product files is -999.
- Surface emissivity is not retrieved over ocean and should be fill values in these cases.
- F04_04 uses the GMAO (Global Modeling Assimilation Office) GEOS-5 products to provide initial guess profiles for temperature and water. GEOS-5 surface (skin) temperature is also used to initiate TES retrievals.
- TES version F04_04 data processed prior to January 1, 2008 uses GMAO GEOS 5.1.0 products. Data processed prior to that date uses GEOS-5.0.1 products. See the

GMAO web site (http://gmao.gsfc.nasa.gov/) for information on the differences in the GMAO products.

- This version of the TES retrieval software utilizes new microwindows in the CO2 band to improve the nadir temperature, water vapor and ozone retrievals. The V003 TES nadir temperature profiles now have 3 to 4 more degrees of freedom for signal as compared to V002. The predicted errors in temperature are reduced by ~0.1 K in the troposphere and ~0.5 K in the stratosphere. The updates also improved the ozone degrees of freedom for signal by ~0.5.
- There is now an emission layer quality flag that screens most cases where the lowest layers of the atmosphere are warmer than the surface (see Section 5.1.1.1)
- TES ozone retrievals will occasionally show anomalously high values near the surface while passing all quality checks. Studies of the V003 ozone data products show that these occur in roughly 2-6% of the TES retrieved profiles. These profiles will show a curved shape in the troposphere ("C-Curve") resulting in high ozone values in the lowest part of the troposphere and low ozone values between 350 and 200 hPa. The unrealistic lapse rates will be seen in some profiles, while adjacent retrieved profiles show no trace of these "C-Curves". These profiles should not be used in scientific analyses (more information in Section 5.1.1.2).
- Constraints on the carbon monoxide retrievals have been loosened for V003 and result in increased degrees of freedom for signal for high latitude measurements. The variability in CO volume mixing ratios have also been seen to increase compared to V002 data.
- TES profiles for chemical species are retrieved in ln(vmr), however the constraint vectors are reported in units of vmr. Users should change the reported constraint vectors to units of ln(vmr) prior in applying them.
- Methane products are improved but should still be used with caution in scientific analyses. Efforts are currently underway to validate the nadir methane retrievals. TES methane retrievals can be better utilized in using an averaging scheme as outlined in (Payne et al., 2008).
- The TES limb product for V04_04 is an improved product over previous versions. Although values are reported on all the TES pressure levels, the averaging kernel indicates where the reported results are influenced by the TES measurements.
- The nadir water products reported in the TES L2 data products usually come from the HDO/H2O retrieval step. There are rare occasions that it comes from the Temperature/H2O/O3 step. The user can determine which step the data is from by looking at the field SurfaceTempvsAtmTemp_QA, if it contains fill (-999), then the data comes from the HDO/H2O step.
- TES limb water vapor data are retrieved only during in scan 4 and not in scans 5 or 6. As a result the water profiles from scans 5 and 6 will contain fill values.
- Emissivity retrievals over desert scenes with strong silicate features can be problematic. Version F03_02 contains an additional land type for our emissivity initial guess, "alluvial sand". This improved the TES retrieved emissivity for target

scenes over the Sahara desert. This land type is currently only for the Sahara desert region in Africa. Consequently the ozone retrievals in the Sahara desert have improved over previous data versions, but the user should be aware that there may be remaining retrieval difficulties for surfaces with high reflectance due to silicate features, which we observe in the Sahara desert, parts of central Australia, and desert regions in Asia.

4.4 TES Version F03_03 Data

It is the first version of TES data products that contain limb data. The current limb retrievals are valid in the stratosphere only. Future versions of TES limb products will contain data that is valid in the troposphere. It also includes minor updates to the nadir data products. This particular version of the TES data products were created using the "Release 9.3" or "R9.3" software and any references to R9.3 data in TES documentation are consistent with F03_03. It may also be referred to as version 2 data.

4.4.1 Known Issues or Advisories for the TES Version F03_03 Data

The TES team has determined a few instances where the most recent data product version should not be used for scientific analysis or used with caution. These are listed below and should be fixed in a future version of the TES data. Also included below are warnings about certain data fields.

- These data contain any advisories seen in the version F04_04 data (Section 4.3.1)
- In this version the L2 profiles are reported on a 67 level grid.
- The TES limb product for V03_03 is a stratospheric product only. Although values are reported on all the TES pressure levels, the averaging kernel indicates where the reported results are influenced by the TES data. The TES limb ozone compares qualitatively well with the TES nadir product. The TES HNO3 product should only be used above 68 mb.
- Potentially large retrieval errors in the lowest layers of the ozone profile for nighttime (descending orbit path) target scenes over land. In some of these night/land cases, a condition can exist where the lowest levels of the atmospheric temperature profile are sufficiently warmer than the surface to create a layer of relatively high thermal contrast. This creates enhanced sensitivity to ozone in emission compared to the ozone in absorption in the layers above it; however, the modeled radiance for the layers in emission would tend to cancel the radiance for the adjacent layer in absorption. The retrieval constraints were not developed for this condition and it can lead to a solution of artificially high ozone.
- Methane products are reported, but should not be (in nearly all cases) used for scientific analysis. Ways of improving the methane product are being tested and should be included in a future version of the TES data.
- The field TotalColumnDensityInitial contains fill values.

- The quantity AIRDENSITY is not in units of molecules cm^{-2} as stated in version 9.0 of the Data Product Specification document. The AIRDENSITY in the product files is in units of molecules m^{-3}
- The nadir geolocation field DominantSurfaceType contains fill values.
- The ancillary file nadir fields OzoneTroposphericColumn, OzoneTroposphericColumnError and OzoneTroposphericColumnInitial contain fill values.
- The units for the constraint vector (ConstraintVector) is incorrectly written to the product file, the units should be 'ln(vmr) or K' not 'vmr or K'.

4.5 TES Version F03_02 Data

This version of the TES data contained significant improvements in scientific data quality over previous versions. It is possible that a data user may find references to TES data releases with a number attached. These data products were created using the "R9.0" software and any references to R9 data in TES documentation are consistent with F03_02. It is also referred to as TES data version V02.

This version of the L2 data has been retrieved from Level 1B (L1B) products that feature a significantly improved radiance calibration (Sarkissian et al., 2005). It represents the best retrieval possible currently available for the L2 products.

4.5.1 Known issues or Advisories for the TES Version F03_02 Data

The TES team has determined a few instances where the most recent data product version should not be used for scientific analysis or used with caution. These are listed below and should be fixed in a future version of the TES data. Also included below are warnings about certain data fields.

- These data contain any advisories seen in the version F04_04 (Section 4.3.1)
- These data contain any advisories seen in the version F03_03 data (Section 4.4.1)
- These TES L2 products do not contain limb data.

4.6 TES Version F02_01 Data

This version of the TES L2 retrieval software was not used for long and there are few TES run IDs processed to this combination of format and data quality. Most importantly these data were not processed using the current L1B radiance calibration. These data were processed with the software version "Release 8" or "R8" and data users may see the version F02_01 data referred to as R8.

4.6.1 Known Issues or Advisories for the TES Version F02_01 Data

In this version the L2 profiles are reported on an 88 level grid.

- These data contain any advisories seen in the version F04_04 (Section 4.3.1)
- These data contain any advisories seen in the version F03_03 data (Section 4.4.1)

- These data contain any advisories seen in the version F03_02 data (Section 4.5.1)
- There are problems retrieving surface emissivity over certain types of desert. This is particularly true over the Sahara regions of Africa, possibly central Australia and parts of Asia. These data should be used with caution.
- There is limited information about the cloud or emissivity retrievals included in the data products files (more information in Section 6.3).
- There is limited information about data quality in this version of the product files.
- Run IDs processed with this version contain no limb retrieval information.

4.7 TES Version F01_01 Data

These were the first TES L2 data products made publicly available. These data were not processed using the current L1B radiance calibration and contains a few processing issues that were resolved for later versions. These data were processed with the software version "Release 7" or "R7" and data users may see the version F01_01 data referred to as R7. It is also referred to as TES data version V01.

4.7.1 Known Issues or Advisories for the TES Version F01_01 Data

In this version the L2 profiles are reported on an 88 level grid.

- These data contain any advisories seen in the version F04_04 (Section 4.3.1)
- These data contain any advisories seen in the version F03_03 data (Section 4.4.1)
- These data contain any advisories seen in the version F03_02 data (Section 4.5.1)
- These data contain any advisories seen in the version F02_01 data (Section 4.6)
- This data have a problem with retrievals over land. There is a software bug that causes problems with high altitude scenes. Scenes with a surface pressure of ~800 hPa or greater are not affected by this bug. High altitude scenes (< 800 hPa) should not be used for this data version.
- There is no information about the cloud or emissivity retrievals included in the data products files.
- There is very limited information about the data quality in the product files.
- Surface temperature retrievals can be problematic due to a software issue.
- Run IDs processed with this version contain no limb retrieval information.
- The Pressure array contains standard pressures for levels below the surface. These should be fill values. The user is advised to look at another field, such as vmr or Altitude, to determine the index of the surface, which is at the first non-fill value.
- Surface temperature and its error are reported from the last step it was retrieved. It should be reported from the step retrieving it with atmospheric temperature, water and ozone. This results in small errors in the reported surface temperatures, and unreliable reported surface temperature errors.

- The data field "SpeciesRetrievalConverged" is underreported due to convergence criteria that are currently set too strictly.
- The data field "LandSurfaceEmissivity" is incorrectly filled in (by initial guess values) for ocean scenes and should be ignored for these scenes.
- The following field is obsolete and contains fill: CloudTopHeight.
- The data field "CloudTopPressure" is sometimes reported as a value greater than the surface pressure. These locations should be interpreted as being cloud-free.

5. TES Data Quality Information

The quality control information provided along with the TES L2 data products have been improved with each data release. The best way to filter data by quality varies for each release and is described below.

5.1 Data Quality Information for Version F04_04 TES Data

The TES retrieval process is non-linear and has the potential to not converge, or converge to a non-global minimum. By studying a larger number of retrievals and comparing results with two different initial conditions, a set of quality flags have been developed and tested that reject about 74% of our bad retrievals and keep about 80% of the "good" retrievals for ozone and temperature. The use of quality flags for other species the filtering percentages are less quantified but should be of a similar order.

A set of quality sub-flags have been developed and are described in the tables below, taken together they make up the "master" quality flag (SpeciesRetrievalQuality). When this flag is set to a value of "1", the data are considered to be of good quality. The master quality flag has been developed for the ozone and temperature retrievals and should not be used for other atmospheric species retrieved by TES. All the numeric values for the quantities used as sub-flags are included in version F03_02 and newer data files. The thresholds for the ozone and temperature master flags are included in Table 5-8, while recommended values for carbon monoxide (Table 5-9) and water (Table 5-10) are also provided below.

Since all the quality control fields are included in the data products files, less stringent quality flags (or fewer flags) could be used if the user wants more of the good cases left in the pool, realizing that more bad cases will also be included. Note that when a flag is set to -999, such as SurfaceEmissMean_QA for ocean scenes, it does not influence the master quality flag.

We retrieve atmospheric parameters in the following steps (0) Cloud detection and possible cloud initial guess refinement (1) T_{ATM}-H_2O-O_3, (2) H_2O/HDO, (3) CH_4, (4) CO. If step (2) does not complete, then the water is reported from step (1) rather than step (2). The user can tell when this occurs because the quality flag CloudVariability_QA (among others) is set to a value different from -999. When this occurs, the user should use the "master" quality flag (SpeciesRetrievalQuality) for H_2O quality. Otherwise, the cutoffs in Table 5-10 should be used for H_2O quality.

A new flag for the HDO retrieval that checks the consistency of the H_2O retrieval from the HDO/H_2O step with the water retrieval from the previous T_{ATM}/H_2O/O_3 step. The condition for this flag is:

- -1 < (H_2O column_1 – H_2O column_2)/(H_2O column error) > 1

where H_2O column_1 is from the T_{ATM}/H_2O/O_3 step and H_2O column_2 is from the H_2O/HDO step.

Finally, since quality temperature retrievals are vital to retrieving trace gases, the quality flag from the temperature is now propagated to subsequent steps and included in the master quality flag for subsequent steps.

5.1.1 Important TES Error Flagging Scenarios

There are two scenarios that should be considered in particular when examining TES ozone and termperature retrievals, one is "Emission layers" and the other is "C-curve" ozone retrievals.

5.1.1.1 Emission Layers

There is a set of conditions designed to screen for "Emission layers" in the lowest part of the atmosphere. This error flag is part of the master quality flag and retrievals that meet these criteria will be flagged as "bad" by the master flag. The two conditions that must be met for an ozone profile to be considered problematic due to an emission layer are:

- Average(T_{ATM}[1^{st} 3 layers]) – TSUR > 1K
- Average(O_3[1^{st} 3 layers] – O_3_initial[1^{st} 3 layers]) > 15 ppb

5.1.1.2 Ozone "C-Curve" Retrievals

The c-curve flag was developed to screen ozone profiles that are likely unphysical and exhibit a c-curve shape with anomalously high ozone near the surface along with anomalously low ozone in the middle troposphere. These profiles were initially found using ozonesonde data for North America and examining coincident TES profiles from Step and Stare special observations. It was noted that adjacent TES profiles would mostly have reasonable agreement with sonde data except for few cases exhibiting the "c-curve" shape. The cause of anomalous c-curve retrievals is being investigated. In the F04_04 data, the number of c-curve profiles for ozone can range from 2-6% of the profiles for a given global survey.

Since sonde data is relatively sparse, it will be difficult to verify where the c-curve cases are actually unphysical. In fact, there are geographical regions where one might expect the c-curve shape, such as North Africa during the winter biomass burning season. Therefore, we recommend the following approach for data analysis with TES V003 ozone profiles.

1) Screen ozone profiles using the general quality flag, degrees of freedom for signal, if needed, and clouds (depending on vertical region of interest).
2) Check for outliers compared to the average and standard deviation. If outliers are significant, try screening with the c-curve to see if results change and behave more reasonably compared to model output or other data.

The test developed to flag to determine if a retrieved TES ozone profile is a c-curve case is based on the following logic:

O3_ret_lo = average of retrieved ozone volume mixing ratios at pressures larger than 700 hPa

O3_init_lo = average of then initial guess ozone volume mixing ratios at pressures larger than 700 hPa

O3_ret_hi = average of retrieved ozone volume mixing ratios at pressures between 200 and 350 hPa

If the ratio (O3_ret_low/O3_init_lo) is greater than 1.6 AND the ratio (O3_ret_low/O3_ret_hi) is greater than 1.4 then the profile can be considered a c-curve case.

Table 5-1 Values for the ten quality "sub-flags" that, taken together, define the master quality flag for ozone and temperature. If all of these criteria are met for an ozone or temperature profile, the master quality flag is set to "1" (good).

Flag	Description	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	The average Cloud Optical Depth (OD) between 975-1200 cm^{-1}. When the optical depth is large, the data results seem to have non-linearity issues.	0	50
CloudVariability_QA	The Cloud OD variability over the retrieved frequencies, scaled by the expected cloud OD error. When the variability is too large, it suggests that the clouds do not exhibit the expected spectral smoothness.	0	2.5
SurfaceEmissMean_QA	The retrieved emissivity bias compared to the *a priori*. If the bias large, it is flagged. Note, when emissivity is not retrieved (over ocean or for limb viewing mode) this is set to -999.	-0.04	0.04
KDotDL_QA	This looks for signal remaining in the radiance residual by calculating the correlation of each Jacobian with the radiance residual, normalized by the Noise Equivalent Spectral Radiance (NESR). The max correlation of all the retrieved parameters is reported.	-0.4	0.4
LDotDL_QA	This looks for signal remaining in the radiance residual by calculating the correlation of the radiance with the radiance residual, normalized by the NESR.	-0.17	0.17
CloudTopPressure	The cloud top pressure. If this is smaller than 90 mb, it is suspect.	90	1300
SurfaceTempvsAtmTemp_QA	Comparison between the boundary layer atmospheric temperature with the surface temperature. When this is very large, the retrieval is suspect. However, the threshold is the same for land and ocean scenes, so a user of ocean scene results may wish to tighten the allowed range. Note when atmospheric temperature and surface temperature are not retrieved this is set to -999.	-25	25

Flag	Description	Minimum Value	Maximum Value
SurfaceTempvsApriori_QA	Comparison between the retrieved and initial surface temperatures. The metrology for surface temperature is expected to be accurate to about 2K. When difference between the result and the initial guess for surface temperature is much larger than this, the retrieval is suspect. Note when surface temperature is not retrieved this is set to -999.	-8	8
RadianceResidualMean	The mean of the difference between observed and fit radiance normalized by the NESR.	-0.2	0.2
RadianceResidualRMS	The rms (root mean square) of the difference between observed and fit radiance normalized by the NESR. Note that this shows a latitudinal variation, peaking in the tropics, for the TATM-H2O-O3 step, but shows no latitudinal variability for CO or H2O-HDO steps.	0.5	1.75
Emission_Layer_Flag	Check to see if there is an emission layer in the lowest part of the atmosphere	-100	1

Table 5-2 Recommended Ranges for TES L2 Quality Flags for Carbon Monoxide

Flag	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	0	50
CloudVariability_QA	0	2
SurfaceEmissMean_QA	-0.06	0.06
KDotDL_QA	-0.45	0.45
LDotDL_QA	-0.45	0.45
CloudTopPressure	90	1300
SurfaceTempvsApriori_QA	-8	8
RadianceResidualMean	-0.5	0.5
RadianceResidualRMS	0.5	1.1

Table 5-3 Recommended Ranges for TES L2 Quality Flags for Water Vapor and HDO

Flag	Minimum Value	Maximum Value
KDotDL_QA	-0.45	0.45
LDotDL_QA	-0.3	0.3
RadianceResidualMean	-0.4	0.4
RadianceResidualRMS	0.5	1.6
H2O_HDO_Quality	-1	1

Table 5-4 Recommended Ranges for TES L2 Quality Flags for Methane

Flag	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	0	50
CloudVariability_QA	0	2
SurfaceEmissMean_QA	-0.06	0.06
KDotDL_QA	-0.45	0.45
LDotDL_QA	-0.3	0.3
CloudTopPressure	90	1300
SurfaceTempvsApriori_QA	-8	8
SurfaceTempvsAtmTemp_QA	-25	25
RadianceResidualMean	-0.3	0.3
RadianceResidualRMS	0.5	1.85

Table 5-5 Recommended Ranges for TES L2 Quality Flags for Limb Temperature and Ozone

Flag	Minimum Value	Maximum Value
KDotDL_QA	-0.34	0.34
LDotDL_QA	-0.75	0.75
RadianceResidualMean	-0.5	0.5
RadianceResidualRMS	0.5	2.0

Table 5-6 Recommended Ranges for TES L2 Quality Flags for Limb Water and HDO

Flag	Minimum Value	Maximum Value
KDotDL_QA	-0.3	0.3
LDotDL_QA	-0.3	0.3
RadianceResidualMean	-0.5	0.5
RadianceResidualRMS	0.5	1.6
H2O_HDO_Quality	-1	1

Table 5-7 Recommended Ranges for TES L2 Quality Flags for Limb Nitric Acid

Flag	Minimum Value	Maximum Value
KDotDL_QA	-0.4	0.4
LDotDL_QA	-0.4	0.4
RadianceResidualMean	-1	1
RadianceResidualRMS	0.5	1.30

5.2 Data Quality Information for Version F03_03 and F03_02 TES Data

The table below describes the quality subflags for the F03_03 and F03_02 data.

The threshold for the RadianceResidualMean quality flag for water is set too tight and will be updated in the next release of the data. When using the F03_02 data the user can use all data in which the absolute value of the RadianceResidualMean flag is less than 0.3 and the RadianceResidualRMS is less than 1.4.

One final note on quality controlling TES data, as mentioned in the warnings section, TES retrievals can occasionally have problems with nighttime scenes over land (emission layer problem). There will be a quality flag for this in the future TES data versions. Until then the user can screen the data by using the criteria:

Average(TATM(i)-TSUR(i)) > 1K and Average(O3(i)-O3 > 15 ppbv (parts per billion by volume) where "Average is over i=0,1,2 for the first non-fill layers in the profile.

Table 5-8 Values for the ten quality "sub-flags" that, taken together, define the master quality flag for ozone and temperature. If all of these criteria are met for an ozone or temperature profile, the master quality flag is set to "1" (good).

Flag	Description	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	The average Cloud optical depth between 975-1300 cm^{-1}. When the optical depth is large, the data results seem to have non-linearity issues.	0	50
CloudVariability_QA	The Cloud OD variability over the retrieved frequencies scaled by the expected cloud OD error. When the variability is too large, it suggests that the clouds do not exhibit the expected spectral smoothness.	0	2
SurfaceEmissMean_QA	The retrieved emissivity bias compared to the *a priori*. If the bias large, it is flagged. Note, when emissivity is not retrieved (over ocean or for limb viewing mode) this is set to -999.	-0.1	0.1
KDotDL_QA	This looks for signal remaining in the radiance residual by calculating the correlation of each Jacobian with the radiance residual, normalized by the NESR. The max correlation of all the retrieved parameters is reported.	-0.17	0.17
LDotDL_QA	This looks for signal remaining in the radiance residual by calculating the correlation of the radiance with the radiance residual, normalized by the NESR.	-0.17	0.17
CloudTopPressure	The cloud top pressure. If this is smaller than 90 mb, it is suspect.	90	1300
SurfaceTempvsAtmTemp_QA	Comparison between the boundary layer atmospheric temperature with the surface temperature. When this is very large, the retrieval is suspect. However, the threshold is the same for land and ocean scenes, so a user of ocean scene results may wish to tighten the allowed range. Note when atmospheric temperature and surface temperature are not retrieved this is set to -999.	-25	25

Flag	Description	Minimum Value	Maximum Value
SurfaceTempvsApriori_QA	Comparison between the retrieved and initial surface temperatures. The metrology for surface temperature is expected to be accurate to about 2K. When difference between the result and the initial guess for surface temperature is much larger than this, the retrieval is suspect. Note when surface temperature is not retrieved this is set to -999.	-8	8
RadianceResidualMean	The mean of the difference between observed and fit radiance normalized by the NESR.	-0.1	0.1
RadianceResidualRMS	The rms of the difference between observed and fit radiance normalized by the NESR. Note that this shows a latitudinal variation, peaking in the tropics, for the TATM-H2O-O3 step, but shows no latitudinal variability for CO or H2O-HDO steps.	0.5	1.75

Table 5-9 Recommended Ranges for TES L2 Quality Flags for Carbon Monoxide

Flag	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	0	50
CloudVariability_QA	0	2
SurfaceEmissMean_QA	-0.2	0.2
KDotDL_QA	-0.45	0.45
LDotDL_QA	-0.45	0.45
CloudTopPressure	90	1300
SurfaceTempvsApriori_QA	-8	8
RadianceResidualMean	-0.5	0.5
RadianceResidualRMS	0.5	1.1

Table 5-10 Recommended Ranges for TES L2 Quality Flags for Water Vapor

Flag	Minimum Value	Maximum Value
KDotDL_QA	-0.45	0.45
LDotDL_QA	-0.45	0.45
RadianceResidualMean	-0.3	0.3
RadianceResidualRMS	0.5	1.4

5.3 Data Quality Information for Version F02_01 TES Data

This version of the data products contains a version of the master quality flag. This flag was optimized to the ozone and temperature retrievals. The values for the sub-flags that went into defining the master quality flag are given in Table 5-11. The version F02_01 data products contain the master quality flag, but not the complete set of the sub-flags, so it will not be possible for a user to create customized quality flags with this version of the data.

Table 5-11 The values for the TES quality sub-flags that go into defining the master quality flag for ozone and temperature for version F02_01. If all of these criteria are met for an ozone or temperature profile, the master quality flag is set to "1" (good).

Flag	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	0	50
CloudVariability_QA	0	2
SurfaceEmissMean_QA	-0.1	0.1
KDotDL_QA	-0.17	0.17
LDotDL_QA	-0.17	0.17
CloudTopPressure	90	1300
SurfaceTempvsAtmTemp_QA	-25	25
SurfaceTempvsApriori_QA	-8	8
RadianceResidualMean	-0.1	0.1
RadianceResidualRMS	0.5	1.5

5.4 Data Quality Information for Version F01_01 TES Data

This version of the products has limited quality control information. The data can be filtered on two values, the radiance residual mean (RadianceResidualMean) which should be less than 1.5 for this version and the radiance residual RMS (RadianceResidualRMS) which should be less than 0.1. This combination of data quality fields should be used for filtering the data for all retrieved species in this version of the TES data.

6. TES Algorithm for Inclusion of Clouds in L2 Retrievals

Clouds are a significant interferent when estimating the distribution of atmospheric trace gases using infrared remote sensing measurements. We have implemented a single-layer non-scattering cloud into our radiative transfer, parameterized as a non-scattering frequency-dependent effective optical depth distribution and a cloud height. These cloud parameters are estimated from spectral data in conjunction with surface temperature, emissivity, atmospheric temperature, and trace gases. From simulations and TES observation comparisons to model fields and atmospheric measurements from AIRS (Atmospheric Infrared Sounder) and TOMS (Total Ozone Mapping Spectrometer), we show that this approach produces accurate estimates and error characterization of atmospheric trace gases for a wide variety of cloud conditions, and introduces no biases into TES estimates of temperature and trace gases for the cases studied (Kulawik et al., 2006b).

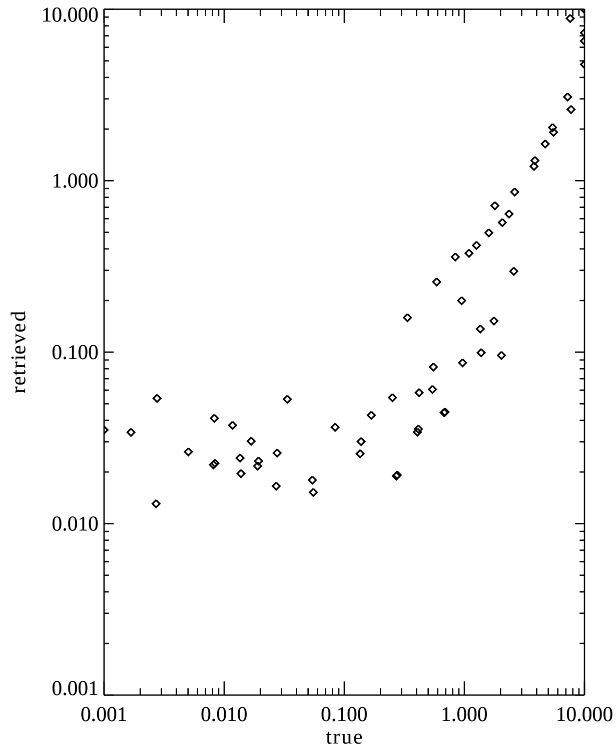
A cloud in the observed atmosphere will reduce sensitivities to trace gases below the cloud, for example an optical depth of 1.0 reduces sensitivity below the cloud to 1/3 of the clear-sky sensitivity (Kulawik et al., 2006b). The sensitivity reduction due to the clouds and all other effects is contained in the averaging kernel, which is provided in the product for each species for each target scene. The averaging kernel describes the sensitivity of the retrieval to the true state (described in more detail in the next section).

As described in (Kulawik et al., 2006b), the cloud optical depth *a priori* is set by the comparison of the brightness temperature in the 11 um window region between TES data and our initial guess atmosphere.

Table 6-1 Cutoffs for Version F04_04

Brightness Temperature (BT) Difference	Cloud Extinction Initial Guess (IG)	Initial Guess Refinement
0.0-0.5	0.0001	No
0.5-1.0	0.001	No
1-2	0.01	No
2-6	0.02	No
6-10	0.8	Yes
10-20	1.3	Yes
20-1000	4	Yes

The initial guess refinement indicates an additional step where only cloud parameters are retrieved. The resulting cloud extinction is more accurate with the new table, as seen in Figure 6-1.



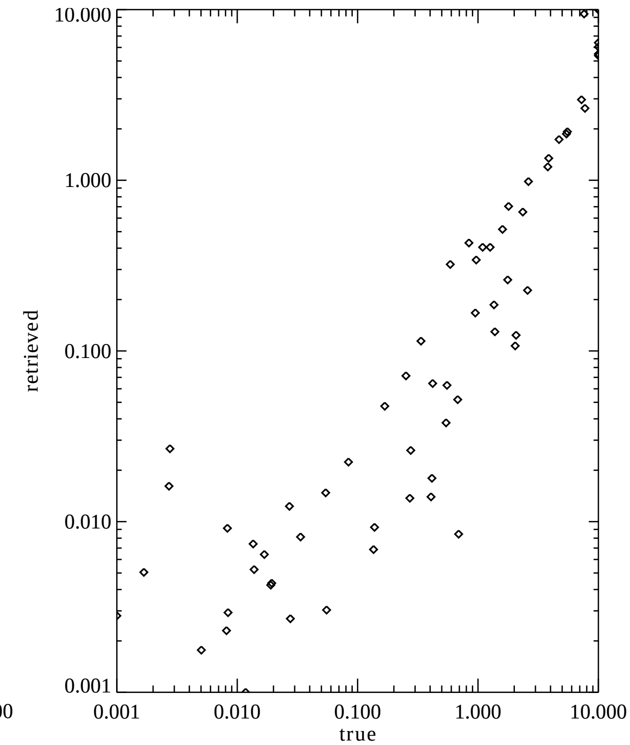


Figure 6-1 Retrieved vs. true optical depth for cloud parameters in a simulated test set. In V002 data (left) the retrieved optical depths bottomed out at about 0.03 OD for this test set. In V003 data (right) the retrieved optical depths better match the true.

6.1 Effective Cloud Property Information Available in the F04_04 and F03_03 Data

The cloud property information provided in these versions of the TES data products is the most extensive. The most important cloud related fields are CloudTopPressure, CloudTopPressureError, CloudEffectiveOpticalDepth, CloudEffectiveOpticalDepthError, and AverageCloudEffOpticalDepth. Cloud effective optical depth and cloud optical depth error fields are discussed in more detail below. The field CloudEffOpticalDepthError contains useable data in this version of the data products.

CloudTopPressure can contain fill data if the retrieved cloud top pressure was below the surface (as happens in some very low optical depth cases). It should be noted also that the CloudTopPressure error is in log space. This error is in log optical depth space, and should be used as described in the data products specification guide.

6.2 Effective Cloud Property Information Available in the F03_02 Data

The AverageCloudEffOpticalDepth is no longer contains fill values as of version F03_02. It is an average over the frequency range 975-1200 cm^{-1}.

6.3 Effective Cloud Property Information Available in the F02_01 data

The version of the data products contains fields: CloudTopPressure, CloudTopPressureError, CloudEffectiveOpticalDepth, and CloudEffectiveOpticalDepthError.

CloudTopPressure can contain fill data if the retrieved cloud top pressure was below the surface (as happens in some very low optical depth cases). It should be noted also that the CloudTopPressure error is in log space.

The CloudEffOpticalDepthError does not contain useable data in this version of the data products.

6.4 Effective Cloud Property Information Available in the F01_01 Data

This version of the data products contains only the fields CloudTopPressure and CloudTopHeight.

There is no cloud optical depth information reported in this version.

The CloudTopHeight field contains fill data.

6.5 Discussion of CloudEffectiveOpticalDepth and CloudEffectiveOpticalDepthError

The CloudEffectiveOpticalDepth and error are retrieved on a fixed frequency grid.

Table 6-2 shows the frequencies that are retrieved and the corresponding species. The cloud top pressure is retrieved whenever the effective optical depth is retrieved. Note that the sensitivity to clouds is not the same at all frequencies, and some will be more influenced by the *a priori*. The errors can be useful to select frequencies that have sensitivity to clouds.

Table 6-2 A List of Atmospheric Species that TES Retrieves as a Function of Frequency

Frequency	F02_01 and F03_02
600	Not retrieved
650	TATM, H2O, O3
700	TATM, H2O, O3
750	TATM, H2O, O3
800	TATM, H2O, O3
850	TATM, H2O, O3
900	TATM, H2O, O3
950	TATM, H2O, O3
975	TATM, H2O, O3
1000	TATM, H2O, O3
1025	TATM, H2O, O3
1050	TATM, H2O, O3

Frequency	F02_01 and F03_02
1075	TATM, H2O, O3
1100	TATM, H2O, O3
1150	TATM, H2O, O3
1200	TATM, H2O, O3
1250	TATM, H2O, O3, then CH4
1300	TATM, H2O, O3, then CH4
1350	TATM, H2O, O3, then CH4
1400	Not retrieved
1900	Not retrieved
2000	CO
2100	CO
2200	CO
2250	Not retrieved

Currently, all of the product files report the effective optical depth from all retrieval steps. Thus, the H2O product file will report effective optical depths for 2000-2200 cm-1, even though that is not retrieved with that species.

From other analysis, we find that the effective optical depth have large uncertainty for effective optical depths less than a few tenths and greater than 2 or so. The small optical depths indicate that a cloud is present, but provide little information on the actual effective optical depth.

6.6 Discussion of CloudTopPressure and CloudTopPressureError

Analysis of the cloud top pressure and cloud optical depths reveals that the cloud top pressure errors are low when the cloud optical depth becomes larger (between a few tenths to ten). For very larger optical depths, which likely correspond to low radiance cases, the cloud top pressure error becomes large again (Figure 6-2).

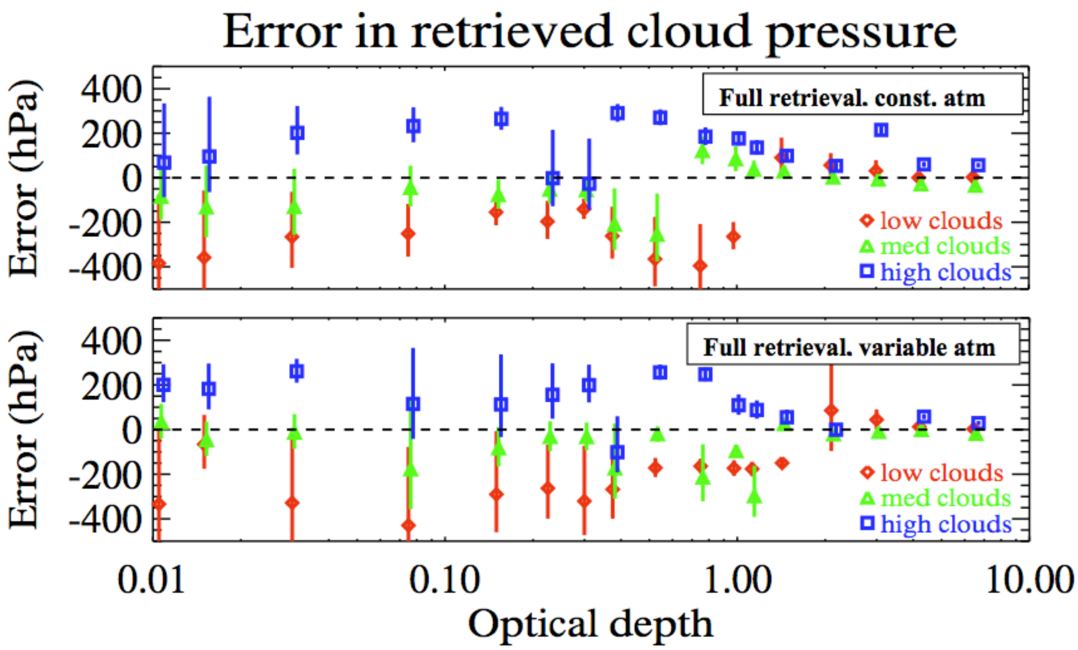


Figure 6-2 Error in the retrieved cloud top pressure (retrieved minus truth) as a function of cloud optical depth for the noise added, full-retrieval simulated cases.

7. TES Data for Assimilation, Inverse Modeling and Intercomparison

7.1 Introduction

The TES retrieval algorithm estimates an atmospheric profile by simultaneously minimizing the difference between observed and model spectral radiances subject to the constraint that the solution is consistent with an *a priori* mean and covariance. Consequently, the retrieved profile includes contributions from observations with random and systematic errors and from the prior. These contributions must be properly characterized in order to use TES retrievals in data assimilation, inverse modeling, averaging, and intercomparison with other measurements. All TES retrievals report measurement and systematic error covariances along with averaging kernel and *a priori* vector. We illustrate how to use these TES data with a comparison of TES ozone retrieval to the GEOS-CHEM chemical transport model.

7.1.1 Characterization of TES Retrievals and Comparisons to Models

If the estimate of a profile is spectrally linear with respect to the true state then the retrieval may be written as (Rodgers, 2000)

$$\hat{\mathbf{y}}_t^i = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\mathbf{y}_t^i - \mathbf{y}_{t,c}^i) + \varepsilon_t^i \qquad (1)$$

where $\hat{\mathbf{y}}_t^i$ is a vector containing the estimated atmospheric state at time *t* and location *i*, $\mathbf{y}_{t,c}^i$ is the constraint vector, $\mathbf{y}_t^i$ is the true atmospheric state, $\mathbf{A}_t^i$ is the averaging kernel, and ε_t^i is the observational error (Bowman et al., 2006).

The estimated atmospheric state may be include the vertical distribution of atmospheric temperature and traces gases as well as effective cloud and surface properties, e.g. surface temperature and emissivity. For the case of trace gas profiles such as carbon monoxide and ozone, the atmospheric state is cast in the logarithm:

$$\mathbf{y}_t^i = \ln \mathbf{x}_t^i \qquad (2)$$

where $\mathbf{x}_t^i$ is a vector whose elements are the vertical distribution of a trace gas in volume mixing ratio.

A retrieval characterized by the averaging kernel and constraint vector can be used to quantitatively compare model fields and *in situ* measurements directly to TES vertical profiles. If the model fields are defined as

$$\mathbf{y}_t^{i,m} = \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t) \qquad (3)$$

where $\mathbf{x}$ is a vector of model fields, $\mathbf{u}$ is a vector of model parameters, e.g. sources and sinks of carbon monoxide, $\mathbf{F}$ is the model operator where the range is defined in terms of the volume mixing ratio for trace gases.

The TES *observation operator* can be written as

$$\mathbf{H}_t(\mathbf{x}_t, \mathbf{u}_t, t) = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\ln \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t) - \mathbf{y}_{t,c}^i) \qquad (4)$$

The logarithm is not applied to model fields associated with atmospheric temperature and surface quantities. From the standpoint of the model, the observations are now expressed in the standard additive noise model, (Jones et al., 2003):

$$\hat{\mathbf{y}}_t^{i,m} = \mathbf{H}(\mathbf{x}_t, \mathbf{u}_t, t) + \varepsilon \qquad (5)$$

The TES observation operator accounts for the bias and resolution of the TES retrieval. Consequently a comparison with TES estimates with a model or *in-situ* data can be described as follows:

$$\hat{\mathbf{y}}_t^{i} - \hat{\mathbf{y}}_t^{i,m} = \mathbf{A}_t^i(\mathbf{y}_t^i - \ln \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t)) + \varepsilon_t^i \qquad (6)$$

The bias in the estimate is removed in the difference. Differences greater than the observational error can be ascribed to differences between the model and the atmospheric state.

The TES ozone retrieval shown in Figure 7-1 was taken from an observation near the island of Sumisu-jima off the coast of Japan on Sept 20, 2004. Figure 7-2 is the averaging kernel calculated for that retrieval. The green profile was calculated by applying the TES observation operator (Equation (4)) to the GEOS-CHEM model field (2x2.5 degrees). The error bars are calculated from standard deviation of the observational error covariance matrix.

For this retrieval, the sensitivity of the retrieval below 800 mb is reduced due to the presence of clouds. Consequently, the GEOS-Chem model profile at those pressure levels relaxes back to the TES *a priori* after the application of the TES observation operator. However, both the GEOS-Chem model and the TES retrieval indicate elevated amounts of ozone in the upper troposphere. The differences between the TES retrieval and GEOS-Chem model are significantly greater than the known observation errors. Therefore, those differences can be attributed to actual differences between the model and the atmospheric state or currently unknown systematic errors within the retrieval.

7.1.2 Mapping (Interpolation) and the Averaging Kernel

The averaging kernel, an example of which is shown in Figure 7-2, is the sensitivity of the retrieved profile to changes in the true state and is composed of 3 matrices:

$$\mathbf{A}_t^i = \frac{\partial \hat{\mathbf{y}}_t^i}{\partial \mathbf{y}_t^i} = \mathbf{M}^i \mathbf{G}_z^i \mathbf{K}_y^i$$

where the mapping (interpolation) matrix is defined as

$$\mathbf{y}_t^i = \mathbf{M}\mathbf{z}_t^i, \qquad \mathbf{M} : \mathbf{R}^M \to \mathbf{R}^N, \;\; M < N \qquad (7)$$

and $\mathbf{z}_t^i$ is a reduced state vector, e.g., a profile on a coarser pressure grid. The mapping matrix projects the retrieval coefficients to the forward model levels. This mapping represents a "hard" constraint on the estimated profile, *.i.e.*, restricts the profile to a subspace defined by **M**.

The second matrix is the gain matrix:

$$\mathbf{G}_z^i = \left((\mathbf{K}_y \mathbf{M})^{\mathrm{T}} \mathbf{S}_n^{-1} \mathbf{K}_y \mathbf{M} + \Lambda \right)^{-1} (\mathbf{K}_y \mathbf{M})^{\mathrm{T}} \mathbf{S}_n^{-1} \qquad (8)$$

The gain matrix projects the TES observed radiances to the TES estimated profiles based on the, hard constraints **M**, the prior and "soft" constraint Λ. The TES spectral Jacobian is defined as

$$\mathbf{K}_y = \frac{\partial \mathbf{L}}{\partial \mathbf{y}} \tag{9}$$

where **L** is the TES forward model, which encompasses both the radiative transfer and the instrumental lineshape (Clough et al., 2006). The averaging kernel is supplied on the forward model pressure grid, which is nominally 88 levels (F01_01 and F02_01) or 67 levels (F03_02 and F03_03) where each level is approximately 1.5 km. The degrees of freedom for signal *(dofs)* for any TES retrieval, which is defined as the trace of the averaging kernel, are significantly less than 87. So, why do we store them on such a fine scale?

- Averaging kernel on a fine pressure scale accommodates a variety of grids, e.g., balloons, tropospheric models, stratospheric models, column trace gas observations
- Averaging kernel can be reduced without loss of information but not vice versa
- Subsequent changes in the retrieval, e.g., changes in **M**, do not change file format.

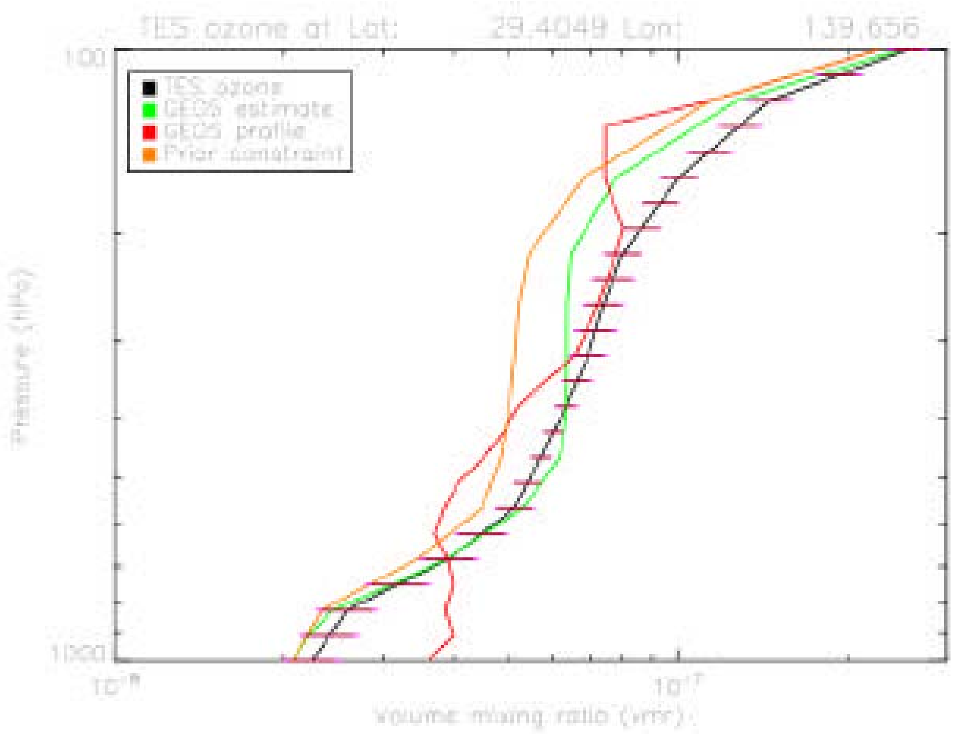


Figure 7-1 TES nadir ozone retrieval taken from an observation near the island of Sumisu-jima off the coast of Japan on Sept 20, 2004. The green profile was calculated by substituting the natural logarithm of a GEOS-CHEM model field x2.5 degrees) into the model TES retrieval equation.

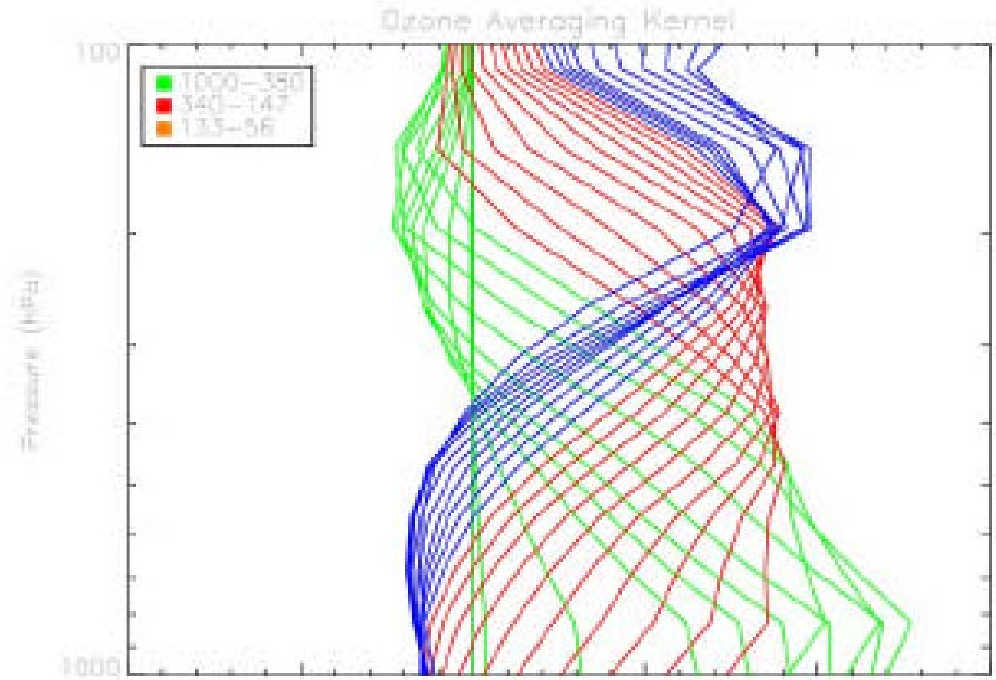


Figure 7-2 TES ozone logarithm averaging kernel from Sumisu-jima observation. Each vertical distribution is the contribution of the true state to the retrieved state at a given pressure level. The 3 colors indicate three pressure regimes for which the averaging kernels have similar distributions.

7.1.3 Examples of Mapping

There are a variety of ways to implement mapping with TES data depending on the application. In the case of some chemistry and transport models or *in situ* measurements, the atmosphere is discretized on coarser pressure levels. A simple linear interpolation in logarithm of vmr can be used to map these coarser levels to the finer TES levels. This mapping is expressed as:

$$\mathbf{M}_{Trop} : \mathbf{R}^{P} \rightarrow \mathbf{R}^{N} \tag{10}$$

where $P < N$. The model retrieval is then

$$\hat{\mathbf{y}}_t^{i,m} = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i (\mathbf{M}_{Trop} \ln \mathbf{F}(\cdot) - \mathbf{y}_{t,c}^i) \tag{11}$$

Note that the product of the averaging kernel and the map can be calculated, which results in a smaller composite matrix. Some instruments produce a column quantity based on scaling a fixed climatological profile. These kinds of data can be compared to the TES retrieval by defining a column vector whose entries are the climatological profile. The mapping looks like

$$\mathbf{M}_c : \mathbf{R} \rightarrow \mathbf{R}^{N} \tag{12}$$

This quantity is scaled by the quantity α leading to the equivalent profile retrieval

$$\hat{\mathbf{y}}_t^i = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i (\ln(\mathbf{M}_c \alpha) - \mathbf{y}_{t,c}^i) \tag{13}$$

This profile can then be compared directly to the TES retrieval.

7.1.4 Conclusions

- TES Level 2 products include, along with retrievals of atmospheric trace gases, averaging kernels, constraint vectors, and error covariance matrices on the forward model levels
- These tools are critical for comparison of TES retrievals to *in situ* sonde measurements, aircraft and satellite measurements, along with comparison to chemical transport models.
- These techniques enable assimilation systems to properly incorporate TES data by characterizing the constraints and biases used in the retrieval without resorting to expensive and non-linear radiative transfer models

7.2 Using TES Data: Comparisons of TES Ozone Profiles with Ozonesondes

The principal source of validation for TES ozone retrievals are comparisons with ozonesonde measurements. In order to make TES-ozonesonde comparisons, we must account for TES measurement sensitivity and the disparities in vertical resolution. This is done by applying the TES averaging kernel and constraint to the ozonesonde profile.

7.2.1 Steps for Comparing TES Retrieved Profiles to Sonde Data

1. Pre-process ozonesonde data
   a. Convert pressure, temperature and O3 to hPa, K, vmr (respectively)
   b. Remove data at duplicate pressure levels (if any). (Duplicate pressures corrupt the mapping to a common pressure grid.)
   c. Append TES initial guess to sonde data in cases where the minimum sonde pressure is > 10 hPa. This is done by scaling the initial guess for O3 and by shifting the initial guess for temperature to the last available sonde values.
   d. Interpolate/extrapolate sonde data to a fixed, fine level pressure grid (800 pressure levels, 180 levels per decade pressure, covering 1260 hPa to 0.046 hPa). This ensures a robust mapping procedure since the pressure grids for sondes are variable and non-uniform.
2. Map sonde profile $\mathbf{x}_{sonde}$ to the pressure level grid used for TES profiles (87 levels covering 1212 hPa to 0.1 hPa) using mapping matrix $\mathbf{M}^*$ which is the pseudo-inverse of the matrix M that interpolates from 87 levels to the fine level grid (800 pressure levels) with $\mathbf{M}^* = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T$.
3. Apply TES averaging kernel, $\mathbf{A}_{xx}$, and *a priori* constraint $\mathbf{x}_{apriori}$:

$$\mathbf{x}_{sonde}^{est} = \mathbf{x}_{apriori} + \mathbf{A}_{xx}[\mathbf{M}^*\mathbf{x}_{sonde} - \mathbf{x}_{apriori}] \qquad (14)$$

   to get the estimated profile $\mathbf{x}^{est}_{sonde}$ that represents what TES would measure for the same air sampled by the sonde. For temperature profiles, the $\mathbf{x}$ is in K. For ozone, water vapor and other trace gases, $\mathbf{x}$ is the natural log of vmr.
4. Compare to TES profile with respect to the measurement and cross-state error terms. The sum of measurement and cross-state errors is labeled the "observational error", which is provided in TES V002 data products.

The total error estimate is given by:

$$\begin{aligned}
&\mathbf{S}_{\tilde{x}} = \text{ (Total error covariance)} \\
&(\mathbf{A}_{xx} - \mathbf{I})\mathbf{S}_a(\mathbf{A}_{xx} - \mathbf{I})^T + \text{ (Smoothing error)} \\
&(\mathbf{A}_{xx_{CS}})\mathbf{S}_a^{x_{CS}x_{CS}}(\mathbf{A}_{xx_{CS}})^T + \text{ (Cross-state error, includes T,H2O)} \\
&\mathbf{M}\mathbf{G}_z\mathbf{S}_n\mathbf{G}_z^T\mathbf{M}^T + \text{ (Measurement error)} \\
&\sum_i \mathbf{M}\mathbf{G}_z\mathbf{K}_\mathbf{b}^i\mathbf{S}_b^i(\mathbf{M}\mathbf{G}_z\mathbf{K}_\mathbf{b}^i)^T \text{ (Systematic errors)}
\end{aligned} \tag{15}$$

where **x** represents the estimated ozone parameters in this case and $\mathbf{M} = \frac{\partial \mathbf{x}}{\partial \mathbf{z}}$ is a linear mapping matrix on pressure levels from retrieval parameters (**z**) to state parameters (**x**). $\mathbf{G}_z$ is the gain matrix, $\mathbf{G}_z = \frac{\partial \mathbf{z}}{\partial \mathbf{F}} = \left(\mathbf{K}_z{}^T\mathbf{S}_n^{-1}\mathbf{K}_z + \Lambda_z\right)^{-1}\mathbf{K}_z{}^T\mathbf{S}_n^{-1}$ where **F** is the forward model radiance, $\mathbf{K}_z$ is the Jacobian matrix, $\mathbf{S_n}$ is the measurement covariance, and Λ_z is the constraint matrix. These give the averaging kernel $\mathbf{A}_{xx} = \mathbf{M}\mathbf{G}_z\mathbf{K}_z\mathbf{M}^{-1}$, which is the sensitivity of the retrieval to the true state. $\mathbf{S_a}$ is the *a priori* covariance (ozone or temperature), $\mathbf{S_a}^{\mathbf{XcsXcs}}$ is the covariance with cross state parameters that are retrieved concurrently. (For ozone, these are atmospheric temperature and water vapor). $\mathbf{S}^i_\mathbf{b}$ is the covariance for the i^{th} forward model systematic error, such as spectroscopic uncertainties, and $\mathbf{K}^i_\mathbf{b}$ are the Jacobian matrices representing the sensitivity of the forward model radiance to these non-retrieved forward model parameters. See (Worden et al., 2004) and (Bowman et al., 2006) for more details on notation and definitions.

8. Overview of Current Data Quality Status

The TES data products have undergone significant validation analyses. The version 2 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 V002 data are available in the TES Validation Report v2.0 (Osterman et al., 2007b). The validation report is available on the Langley ASDC web site. There also have been 13 papers submitted for inclusion in a future special issue of Journal of Geophysical Research – Atmospheres dealing with Aura validation. Accepted papers as of July 31, 2008, are listed below in Section 9. It should be noted that the TES nadir methane and all limb products are considered to be "beta" validated, meaning that data is basically useful for gaining familiarity with the TES products and the best way to use them.

The following subsections give an overview of the current data quality of the TES V003 (F04_04) data products.

8.1 Data Quality and Validation Status for TES Products

8.1.1 TES L1B Radiances

TES L1B V002 and V003 data products are a significant improvement over V001 (Beta release). Nadir spectral radiance validation results have been published in (Shephard et al., 2008a). Several systematic errors have been resolved giving much better agreement with Aqua-AIRS radiance measurements of the same homogenous target scenes (see below). The error estimates given below are representative of TES nadir data. Errors specific to each target spectrum are available within the data products.

Precision estimates are given in the NESR (Noise Equivalent Spectral Radiance) part of the L1B product which is available with each target spectral radiance. The NESR is estimated for each measured spectrum using the noise extracted from the spectral range outside the signal region allowed by the TES optical filter used for the measurement. The NESRs have not changed significantly due to algorithm improvements, however, data acquired after December 7, 2005 (TES Run ID 3202 and higher) have better NESRs (around 50 $nW/cm^2/sr/cm^{-1}$) due to improved optical alignment following the warm up of the TES optical bench to a higher operating temperature.

Table 8-1 TES Average Single Detector, Single Scan Nadir NESR Values

Filter	Frequency Range (cm^{-1})	Nadir NESR ($nW/cm^2/sr/cm^{-1}$)
2B1	650 – 930	700
1B2	920 – 1160	200
2A1	1090 – 1350	150
1A1	1890 – 2260	100

Based on our validation with the Atmospheric Infrared Sounder (AIRS) instrument on the NASA Aqua satellite and our L2 retrievals, we estimate our systematic errors to be less that 0.5 K in brightness temperature. A known remaining error source is due to velocity jitter that affects our interferogram sampling. This sampling error produces the largest uncertainties (<1%) near the edges of our frequency filter bands. To mitigate this error, we suggest only using L1B data that is about 30 cm^{-1} away from the spectral range boundaries, for example, 950-1130 cm^{-1} for filter 1B2. Recommended spectral ranges for L2 data are listed in Table 3 of (Shephard et al., 2008a) for each filter.

We have compared nadir TES L1B calibrated radiance spectra to AIRS radiances by first convolving TES spectra with the AIRS spectral response function (SRF). Mean and RMS AIRS-TES differences in observed brightness temperature for homogenous targets (as determined by TES) are <0.5 K. Specifically, Shephard et al. (2008a) reported that mean AIRS-TES differences are <0.3 K at brightness temperatures of 290-295 K, and <0.5 K at 265-270 K.

We see similar (small) differences in our comparisons to S-HIS (Scanning - High Resolution Spectrometer) measurements taken from the WB-57 aircraft during the AVE (Aura Validation Experiment) Oct-Nov. 2004, and during CR-AVE (Costa Rica Aura Validation Experiment), Jan-Feb 2006. Shephard et al. (2008a) reported that the mean and RMS differences between S-HIS and TES, adjusted for geometrical differences, are <0.3 K at brightness temperatures of 290-295 K and <0.4 K at 265-270 K.

8.1.2 Nadir Ozone

Statistical comparisons of V002 TES ozone profiles to ozonesondes show that TES has a high bias of 3-10 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. It is expected that the bias in TES ozone profiles compared to sondes is decreased in the upper troposphere for the V003 data. Comparisons of TES data to measurements from the NASA (National Aeronautics and Space Administration) Langley Research Center DIAL (Differential Absorption Lidar) instrument show a similar high bias in the troposphere of between 5-15% (Richards et al., 2008). Comparisons of stratospheric ozone columns calculated from the TES data to similar columns from MLS (Microwave Limb Sounder) ozone show good agreement with TES biased high by 2-5 DU (Dobson Units) (Osterman et al., 2008).

8.1.3 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 to the aircraft in-situ measurements during INTEX-B (International Chemical Transport Experiment) 2006, AVE (Aura Validation Experiment, Houston, TX) 2004, CR-AVE (San Jose, Costa Rica) 2006, and PAVE (Polar Aura Validation Experiment) 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 (Measurement of Pollution in The Troposphere) 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.

8.1.4 Nadir Atmospheric Temperature

The V003 TES temperature retrievals have been improved due the use of the CO2 ν2 band with improved spectroscopy in the retrieval software. The V003 TES nadir temperature profiles now have 3 to 4 more degrees of freedom for signal as compared to V002. The predicted errors in temperature are reduced by ~0.1 K in the troposphere and ~0.5 K in the stratosphere. Comparisons to RS90 and RS92 radiosondes from the NCEP database show that TES V002 temperature retrievals are biased low by ~1K in the upper troposphere and stratosphere. This bias has been reduced to 0.5 K in the V003 data. The sonde comparisons also show a cold bias of 1 to 2 K at 400 hPa for both V002 and V003 data. Steps are underway to improve this bias further.

8.1.5 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 AMSR-E (Advanced Microwave Scanning Radiometer) 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.

8.1.6 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.

8.1.7 Nadir Methane

We are currently working to characterize and validate the methane product. Work by Vivienne Payne at AER has demonstrated a way of using the TES methane product doing some post processing to focus on the regions of peak sensitivity (Payne et al., 2008). Preliminary comparisons utilizing very limited data sets have revealed a high bias in the TES methane product of ~5%. Preliminary comparisons with ground-based up-looking IR Fourier transform spectrometer data (available through from the international Network for the Detection of Stratospheric Change: http://www.ndsc.ncep.noaa.gov/organize/) show TES is higher by 0-10% in the total column amount (TES vertical sensitivity has not yet been folded into this calculation). Compared with a profiles obtained from in-situ data taken during the 2006 INTEX-B campaign, TES was often ~5% higher than the in-situ data in the 200-400 hPa range.

8.1.8 Nadir Surface Temperature (Sea Surface Temperature)

TES retrieves surface (skin) temperature as standard product. Over ocean this amounts to a sea surface temperature (SST). The TES SST compared to Reynolds Optimally Interpolated (daily) SST is within 1.2 K (RMS) and has a best fit Gaussian width (done to eliminate a small set of cold/cloud contaminated outliers) of 0.6 K for target scenes with effective cloud optical depth less than 0.05. For all target scenes Examined the TES SST is within 1.77 K (RMS) with a Gaussian width of 0.7 K. For TES SST the master data quality flag eliminates about 20-25% of the target scenes, however the RMS and Gaussian widths of TES vs. ROI are the same, 1.77 K (RMS) and 0.7 K.

8.1.9 Limb Ozone

Limb ozone compares well to TES nadir ozone when the averaging kernel is considered in the comparisons.

8.1.10 Limb Atmospheric Temperature

Limb temperature has been compared to model predictions from GMAO GEOS-5. For a TES global survey on September 20-21, 2004, the TES limb temperature shows a -0.15K bias (TES low) and 0.6 rms difference compared to the GMAO GEOS-5 values in the troposphere, and between 0 and 1.6K bias (TES high) with about a 1-1.5 K rms difference in the stratosphere.

8.1.11 Limb Nitric Acid

Limb nitric acid has been compared to data from in situ aircraft instruments, aircraft FTIR (Fourier Transform Infrared) and other satellite instruments such as EOS MLS. Comparisons to these datasets show TES retrievals provide reasonable results above 100 hPa and the data show expected global features, such as the stratospheric depletion in the southern polar winter.

8.1.12 Limb Water Vapor

Limb water and HDO in general show low sensitivity and are mainly used as interfering species when retrieving temperature, ozone, and nitric acid.

9. Supporting Documentation

If after using this document, the data user still has further questions, the following documents provide further information on the TES instrument and data. TES documentation and publications are available at the TES web site: http://tes.jpl.nasa.gov/docsLinks/index.cfm . The documentation is also available at the Langley ASDC site: http://eosweb.larc.nasa.gov/PRODOCS/tes/table_tes.html .

Description of the TES instrument can be found in the following publications:

[Beer, 2006] Beer, R., TES on the Aura Mission: Scientific Objectives, Measurements, and Analysis Overview, *IEEE Trans. Geosci. Remote Sensing*, 44, 1102- 1105, May 2006.

[Beer et al., 2001] Beer, R., T. A. Glavich, and D. M. Rider, Tropospheric emission spectrometer for the Earth Observing System's Aura satellite, *Applied Optics*, 40, 2356-2367, 2001.

[Beer, 1999] Beer, R., TES Scientific Objectives & Approach, Goals & Requirements, Revision 6.0, JPL D-11294, April 14, 1999.

Information on TES L1B radiances including the improved L1B calibration are given in the following:

[Shephard et al., 2008a] Shephard, M. W., H. M. Worden, K. E. Cady-Pereira, M. Lampel, M. Luo, K. W. Bowman, E. Sarkissian, R. Beer, D. M. Rider, D. C. Tobin, H. E. Revercomb, B. M. Fisher, D. Tremblay, S. A. Clough, G. B. Osterman, M. Gunson, Tropospheric Emission Spectrometer Nadir Spectral Radiance Comparisons, *J. Geophys. Res.*, 113, D15S05, doi:10.1029/2007JD008856, April 22, 2008a.

[Sarkissian et al., 2005] Sarkissian, E. et al., TES Radiometric Assessment, AGU Fall 2005, A41A-0007, December 2005.

[Worden and Bowman, 1999] Worden, H.M. and K. W. Bowman., TES Level 1B Algorithm Theoretical Basis Document, Version 1.1, JPL-D16479, October, 1999.

A description of the format and contents of the TES data products are provided in the data product specification documents:

[Lewicki, 2007] Lewicki, S., TES Science Data Processing Standard and Special Observation Data Products Specifications, Version 10.13, JPL D-22993, April 26, 2007, for public released data, software release 10.

[Lewicki, 2005a] Lewicki, S., TES Science Data Processing Standard and Special Observation Data Products Specifications, Version 9.0, JPL D-22993, December 13, 2005a, for public released data, software release 9.

[Lewicki, 2005b] Lewicki, S., TES Science Data Processing Standard and Special Observation Data Products Specifications, Version 8.0, JPL D-22993, July 7, 2005b, for public released data, software release 8.

[Lewicki, 2005c] Lewicki, S., TES Science Data Processing Standard and Special Observation Data Products Specifications, Version 7.0, JPL D-22993, March 17, 2005c, for public released data, software release 7.

The following list of documents and publications provides information on the algorithms used in producing the data and different aspects of the quality of the TES data products.

[Osterman, 2004] Osterman, G.B., Editor, TES Level 2 Algorithm Theoretical Basis Document, Version 1.16, JPL D-16474, June 30, 2004.

[Kulawik et al., 2006a] Kulawik, S. S., H. Worden, G. Osterman, M. Luo, R. Beer, D. Kinnison, K.W. Bowman, J. Worden, A. Eldering, M. Lampel, T. Steck, C. Rodgers, TES Atmospheric Profile Retrieval Characterization: An Orbit of Simulated Observations, *IEEE Trans. Geosci. Remote Sensing*, 44, 1324-1333, May 2006a.

[J. Worden et al., 2004] Worden, J., S. Sund-Kulawik, M.W. Shephard, S. A. Clough, H. Worden, K. Bowman, A. Goldman, Predicted errors of tropospheric emission spectrometer nadir retrievals from spectral window selection, *J. Geophys. Res.*, Vol. 109, No. D9, D09308, 10.1029/2004JD004522, May 15, 2004.

Information on how TES handles clouds in the L2 retrieval process can be found in the following:

[Eldering et al., 2008] Eldering, A., S. S. Kulawik, J. Worden, K. Bowman, and G. Osterman, Implementation of Cloud Retrievals for TES Atmospheric Retrievals - part 2: characterization of cloud top pressure and effective optical depth retrievals, *J. Geophys. Res.*, 2008, in press.

[H. Worden et al., 2007] Worden, H. M., J. Logan, J. R. Worden, R. Beer, K. Bowman, S. A. Clough, A. Eldering, B. Fisher, M. R. Gunson, R. L. Herman, S. S. Kulawik, M. C. Lampel, M. Luo, I. A. Megretskaia, G. B. Osterman, M. W. Shephard, Comparisons of Tropospheric Emission Spectrometer (TES) ozone profiles to ozonesodes: Methods and initial results, *J. Geophys. Res - Atmospheres*, 112, D03309, doi:10.1029/2006JD007258, February 15, 2007.

[Kulawik et al., 2006b] Kulawik, S.S., J. Worden, A. Eldering, K.W. Bowman, M. Gunson, G. B. Osterman, L. Zhang, S.A. Clough, M. W. Shephard, R. Beer, Implementation of cloud retrievals for Tropospheric Emission Spectrometer (TES) atmospheric retrievals - part 1. Description and characterization of errors on trace gas retrievals, *J. Geophys. Res - Atmospheres*, 111, D24204, doi:10.1029/2005JD006733, December 22, 2006b.

Information on using TES data for data comparisons, assimilation and inverse modeling can be found in the following:

[Kulawik et al., 2008] Kulawik, S. S., K. W. Bowman, M. Luo, C. D. Rodgers, and L. Jourdain, Impact of nonlinearity on changing the a priori of trace gas profiles estimates from the Tropospheric Emission Spectrometer (TES), *Atmos. Chem. Phys. Discuss.*, 8, 1261-1289, 2008.

[Parrington et al., 2008] Parrington, M., D. B. A. Jones, K. W. Bowman, L. W. Horowitz, A. M. Thompson, D. W. Tarasick, and J. C. Witte, Estimating the summertime tropospheric ozone distribution over North America through assimilation of observations from the tropospheric emission spectrometer, *J. Geophys. Res.*, 2008, in press.

[Bowman et al., 2006] Bowman, K.W., Clive D. Rodgers, Susan Sund-Kulawik, John Worden, Edwin Sarkissian, Greg Osterman, Tilman Steck, Ming Lou, Annmarie Eldering, Mark Shepherd, Helen Worden, Michael Lampel, Shepherd Clough, Pat Brown, Curtis Rinsland, Michael Gunson, Reinhard Beer, Tropospheric Emission Spectrometer: Retrieval Method and Error Analysis, *IEEE Trans. Geosci. Remote Sensing*, 44, 1297- 1307, May 2006.

[Jones et al., 2003] Jones, D.B.A., K.W. Bowman, P.I. Palmer, J.R. Worden, D.J. Jacob, R.N. Hoffman, I. Bey, and R. M. Yantosca. Potential of observations from the Tropospheric Emission Spectrometer to constrain continental sources of carbon monoxide. *J. Geophys. Res.-Atmospheres*, Vol.108, No. D24, 4789, 10.1029/2003JD003702, 2003.

[J. Worden et al., 2004] Worden, J., S. Sund-Kulawik, M.W. Shephard, S. A. Clough, H. Worden, K. Bowman, A. Goldman, Predicted errors of tropospheric emission spectrometer nadir retrievals from spectral window selection, *J. Geophys. Res.*, Vol. 109, No. D9, D09308, 10.1029/2004JD004522, May 15, 2004.

[H. Worden et al., 2007] Worden, H. M., J. Logan, J. R. Worden, R. Beer, K. Bowman, S. A. Clough, A. Eldering, B. Fisher, M. R. Gunson, R. L. Herman, S. S. Kulawik, M. C. Lampel, M. Luo, I. A. Megretskaia, G. B. Osterman, M. W. Shephard, Comparisons of Tropospheric Emission Spectrometer (TES) ozone profiles to ozonesodes: Methods and initial results, *J. Geophys. Res. - Atmospheres*, 112, D03309, doi:10.1029/2006JD007258, February 15, 2007.

Information on the initial validation of TES data products can be found in the following:

[Payne et al., 2008] Payne, V. H., S. A. Clough, M. W. Shephard, R. Nassar, J. A. Logan, Information-centered representation of retrievals with limited degrees of freedom for signal: Application to methane from the Tropospheric Emission Spectrometer, submitted to *J. Geophys. Res* ., 2008.

[Nassar et al., 2008] Nassar, R., J. A. Logan, H. M. Worden, I. A. Megretskaia, K. W. Bowman, G. B. Osterman, A. M. Thompson, D. W. Tarasick, S. Austin, H. Claude, M. K. Dubey, W. K. Hocking, B. J. Johnson, E. Joseph, J. Merrill, G. A. Morris, M. Newchurch, S. J. Oltmans, F. Posny, F. J. Schmidlin, H. Vomel, D. N. Whiteman, J. C. Witte, Validation of Tropospheric Emission Spectrometer (TES) Nadir Ozone Profiles Using Ozonesonde Measurements, *J. Geophys. Res.*, 113, D15S17, doi:10.1029/2007JD008819, May 7, 2008.

[Osterman et al., 2008] Osterman, G., S.S. Kulawik, H.M. Worden, N.A.D. Richards, B.M. Fisher, A. Eldering, M.W. Shephard, L. Froidevaux, G. Labow, M. Luo, R.L. Herman, K.W. Bowman, and A. M. Thompson, Validation of Tropospheric Emission Spectrometer (TES) Measurements of the Total, Stratospheric and Tropospheric Column Abundance of Ozone, *J. Geophys. Res.*, 113, D15S16, doi:10.1029/2007JD008801, May 7, 2008.

[Shephard et al., 2008a] Shephard, M. W., H. M. Worden, K. E. Cady-Pereira, M. Lampel, M. Luo, K. W. Bowman, E. Sarkissian, R. Beer, D. M. Rider, D. C. Tobin, H. E. Revercomb, B. M. Fisher, D. Tremblay, S. A. Clough, G. B. Osterman, M. Gunson, Tropospheric Emission Spectrometer Nadir Spectral Radiance Comparisons, *J. Geophys. Res.*, 113, D15S05, doi:10.1029/2007JD008856, April 22, 2008a.

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[Lopez et al., 2008] Lopez, J. P., M. Luo, L. E. Christensen, M. Loewenstein, H. Jost, C. R. Webster, and G. Osterman, TES carbon monoxide validation during two AVE campaigns using the Argus and ALIAS instruments on NASA's WB-57F, *J. Geophys. Res.*, doi:10.1029/2007JD008811, 2008, in press.

[Richards et al., 2008] Richards, N. A. D., G. B. Osterman, E. V. Browell, J. W. Hair, M. Avery and Q. Li, Validation of Tropospheric Emission Spectrometer (TES) Ozone Profiles with Aircraft

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A complete list of TES related documents and publications can be found on the TES "Documents & Links" website http://tes.jpl.nasa.gov/docsLinks/index.cfm .

Appendices

A. Acronyms

AIRS	Atmospheric Infrared Sounder
AMSR	Advanced Microwave Scanning Radiometer
ASDC	Atmospheric Science Data Center
AVE	Aura Validation Experiment
BT	Brightness Temperature
CH_4	Methane, Natural Gas
CO	Carbon Monoxide
CO2	Carbon Dioxide
CR-AVE	Costa Rica Aura Validation Experiment
DIAL	Differential Absorption Lidar
DOFS	Degrees of Freedom for Signal
DPS	Data Products Specification
DU	Dobson Units
EOS	Earth Observing System
ESDT	Earth Science Data Type
FTIR	Fourier Transform Infrared
FTP	File Transfer Protocol
FTS	Fourier Transform Spectrometer
GEOS	Global Earth Observing System
GMAO	Global Modeling Assimilation Office
H2O	Dihydrogen Monoxide (Water)
HDF	Hierarchical Data Format
HDO	Hydrogen Deuterium Monoxide ("Heavy Water")
HIRDLS	High Resolution Dynamics Limb Sounder
HIS	High Resolution Interferometer Sounder
HNO3	Nitric Acid
ID	Identification Number
IEEE	Institute of Electrical and Electronics Engineers

IG	Initial Guess
INTEX	International Chemical Transport Experiment
JPL	Jet Propulsion Laboratory
K	Kelvin
L1B	Level 1B
L2	Level 2
MLS	Microwave Limb Sounder
MOPITT	Measurement Of Pollution In The Troposphere
NASA	National Aeronautics and Space Administration
NCEP	National Centers for Environmental Prediction
NESR	Noise Equivalent Spectral Radiance
O3	Ozone
OD	Optical Depth
PAVE	Polar Aura Validation Experiment
ppb	parts per billion
ppbv	parts per billion by volume
RMS	Root-Mean-Square
Run ID	TES Run Identification Number
SRF	Spectral Response Function
SST	Sea Surface Temperature
TBD	To Be Determined
TBR	To Be Released, To Be Reviewed, To Be Revised
TES	Tropospheric Emission Spectrometer
TOMS	Total Ozone Mapping Spectrometer
vmr	volume mixing ratio