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Atmospheric Measurement Techniques
Discussions

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Characterization and Evaluation of AIRS-Based Estimates of the Deuterium Content of Water Vapor

Abstract: Single pixel, tropospheric retrievals of HDO and H_2O concentrations are retrieved from Atmospheric Infrared Sounder (AIRS) radiances using the optimal estimation algorithm developed for the Aura Tropospheric Emission Spectrometer (TES) project. These retrievals are evaluated against co-located TES observations taken between 2006 through 2010. We evaluate the error characteristics and vertical sensitivity of AIRS measurements corresponding to five days of TES data (or 5 global surveys) during the N. Hemisphere summers between 2006 and 2010 (~600 co-located comparisons per day). We find that the retrieval characteristics of the AIRS deuterium content measurements have similar vertical resolution and uncertainty in the middle-troposphere as TES but with slightly less sensitivity in the lower-most troposphere, with a typical degrees-of-freedom (DOFS) in the tropics of 1.5. The difference in sensitivity to the lower-most troposphere is mostly likely due to the reduced spectral resolution as previous studies found that spectral resolution was the primary factor, relative to signal-to-noise, affecting the vertical resolution of nadir sounding retrievals (Worden *et al*. 2004). The calculated measurement uncertainty is ~30 per mil (parts per thousand relative to the deuterium composition of ocean water) for a tropospheric average between 750 and 350 hPa, the altitude region where AIRS is most sensitive. Comparison with the TES data suggest that the calculated and actual uncertainty of a single target AIRS HDO/H_2O measurement ~30 per mil. Comparison of AIRS and TES data between 30 S and 50 N suggest that the AIRS data is biased low by ~-2.6 per mil with a latitudinal variation of ~7.8 per mil. This latitudinal variation is consistent with the accuracy of TES data as compared to in situ measurements, suggesting that both AIRS and TES have similar accuracy.

1) Introduction:

In this paper we demonstrate a retrieval algorithm, based upon the Aura TES optimal estimation retrieval algorithm (e.g. Worden *et al*. 2012) that can provide robustly characterized measurements of the deuterium content of water vapor (HDO and H_2O) from the AIRS and TES measurements. Our goal is to create a multi-decadal Earth Science Data Record (ESDR) using the AIRS data, as the TES global record spans ~6 years and the AIRS data span 15+ years starting in 2002. This ESDR could potentially be used for evaluating the changing water cycle (e.g. Worden *et al*. 2007a; Frankenberg *et al*. 2010; Risi *et al*. 2012; Frankenberg *et al*. 2013; Galewsky *et al*., 2016; Bailey *et al*., 2017; Wright *et al*., 2017) and its coupling to the carbon cycle (e.g. Zhou *et al*., 2014; Wright *et al*. 2017). The algorithm we use also jointly retrieves methane from the AIRS radiances (e.g. Xiong *et al*. 2008, 2013) and we will use these methane retrievals for the purpose of creating a joint AIRS / TES record of CH_4 and for quantifying lower-tropospheric methane (Worden *et al*., 2015) by combining these data with total column methane measurements (Worden *et al*., 2013 Worden *et al*., 2017). However, the evaluation and validation of these methane retrievals will be discussed in a subsequent paper.

We first characterize the vertical resolution and uncertainties for estimates of HDO and H_2O using AIRS radiance observations corresponding to summertime TES global survey's between 2006 through 2010 which is the time period when TES observations sample the (near) global atmosphere and the calibration approach for TES remained the same. We then compare the AIRS and TES data to evaluate and quantify the calculated uncertainties of the AIRS data. A follow-on paper will compare these AIRS data to aircraft data taken during the NASA ORACLES (ObseRvations of Aerosols above CLouds and their intEractionS) campaign.

2) Description of AIRS and TES instruments

The AIRS instrument is a nadir-viewing, scanning infrared spectrometer (Aumann *et al*. 2003; Pagano *et al*., 2003; Irion *et al*. 2018; DeSouza-Machado *et al*. 2018) that is onboard the NASA Aqua satellite and was launched in 2002. AIRS measures the thermal radiance between approximately 3-12 microns with a resolving power of approximately 1200. For the 8 micron spectral range used for the HDO/H_2O retrievals, the spectral resolution is ~1 cm^{-1} with a gridding of ~0.5 cm^{-1} and the signal-to-noise (SNR) ranges from ~400 to ~1000 over the 8 micron region for a typical tropical scene. A single footprint has a diameter of ~15 km in the nadir; given the ~1250 km swath, the AIRS instrument can measure nearly the whole globe in a single day. The Aqua satellite is part of the "A-Train" that consists of multiple satellites, including TES, in a sun-synchronous orbit at 705 km with an approximately 1:30 pm equator crossing-time.

The A-Train also consists of the Aura TES instrument which is a Fourier Transform Spectrometer that originally was designed to measure the thermal infrared (IR) radiances both in the limb and nadir viewing in order to obtain vertically resolved trace gas profiles of ozone, CO, CH_4, HDO and H_2O, and several ozone pre-cursors such as ammonia, methanol, and PAN, (e.g. Beer *et al.,* 2001; Worden *et al.,* 2004; Worden *et al*. 2006; Luo *et al.,* 2007; Beer *et al*. 2008; Worden *et al.,* 2012; Payne *et al*. 2014). Several of these trace gases, such as CO, CH_4, and ammonia have been quantified using AIRS radiances (e.g. McMillan *et al.,* 2005; Xiong *et al*. 2008; Warner *et al.,* 2016). In comparison to the AIRS instrument, TES has a spectral resolution of ~0.12 cm^{-1} (apodized) with a spectral gridding of 0.06 cm^{-1}. The SNR is ~300 in the 8 microns spectral region. The Aura TES instrument, after the summer of 2005, observes one nadir scene every 100 km along the orbit path. The effective length of the record is approximately five years, between September 2005 through November 2009, after which instrument degradation problems resulted in interrupts and a decrease in sampling. The AIRS instrument has nearly one thousand times the sampling of TES and near continuous operation between 2002 through the present and therefore can be used to construct several composition based Earth System Data Records (ESDR's).

3) Description of Radiative Transfer Forward Model

The radiative transfer forward model used for this work is the Optimal Spectral Sampling (OSS) fast radiative transfer model (RTM) (Moncet et al., 2015; Moncet et al., 2008). The OSS approach is integrated in the operational Cross-Track Infrared Sounder (CrIS, Han et al. 2013) processing system (Divarkala et al., 2014) and has also been utilized for trace gas retrievals from CrIS (e.g. Shephard and Cady-Pereira, 2015). OSS uses a series of approximations tailored to a

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specific frequency range and spectral resolution to increase the radiative transfer calculation performance by approximately a factor of 20-100 relative to a line-by-line calculation (http://rtweb.aer.com). OSS can be trained to user-defined accuracy relative to the line-by-line model used for training. Here, the training threshold was set to 20 % of the AIRS noise level. The line-by-line model used as a reference in the training and to build the absorption coefficient look-up tables (LUTs) used by the fast RTM is the Line-By-Line Radiative Transfer Model (LBLRTM) (Clough et al., 2005; Alvarado et al., 2013). The OSS version used in this work is based on LBLRTM v12.4, using the TES_v2.0 spectroscopic line parameter database. The TES_v2.0 line parameter database follows the HITRAN 2012 compilation (Rothman et al., 2013]), with the following exceptions:

- H_2O positions and intensities are taken from the aer_v_3.4 line parameter database (http://rtweb.aer.com), closely following the measured and calculated values published in Coudert et al. (2008).
- CH_4 includes first order line mixing coefficients (as supplied in the aer_v_3.4 line parameter database). These were calculated using the approach of Tran et al. (2006).
- CO_2 line parameters are from the database of Lamouroux et al. (2015). This database takes most of its line positions, intensities, and lower state energies from the HITRAN 2012 database, but the values for air-broadening half-widths and their temperature dependences are adjusted from the HITRAN 2012 values to be consistent throughout the bands, and the air-induced pressure shifts (not given for a majority of transitions in HITRAN 2012) were added. The TES_v2.0 database includes first order line mixing coefficients (as supplied in the aer_v_3.4.1 line parameter database), calculated using the software of Lamouroux et al. (2015).

Further information on the AER line parameter databases can be found at http://rtweb.aer.com. OSS is adapted for use with AIRS radiances using a version of the v4 AIRS spectral response function (SRF) (Strow et al., 2003) that is interpolated to a uniform grid of 0.004 cm^{-1} centered on the channel center frequencies. The OSS radiative transfer code provides speedup of 20-100x over the original TES operational radiation transfer model (Clough *et al*., 2006).

4) Description of Retrieval Approach

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The optimal estimation algorithm used in this analysis for quantifying CH_4, HDO, H_2O, temperature, cloud properties, and emissivity is extensively discussed in Worden et al. (2004), Bowman et al. (2006), and Worden et al (2012). We therefore refer the reader to those papers for a description of the retrieval algorithm, with a suggestion that they start with the Worden *et al*. (2012) paper, and will summarize the retrieval approach here. This retrieval algorithm, now called the MUlti-SpEctra, MUlti-SpEcies, MUlti-Sensors (MUSES) algorithm (Worden et al., 2007b; Fu et al., 2013, 2016, 2018; Luo et al., 2013; Worden et al., 2013), can use radiances from multiple instruments including TES, CrIS, OMI, OMPS, TROPOMI, and MLS to quantify and characterize geophysical observables appropriate for the corresponding radiance.

Briefly, we simultaneously estimate not just CH_4, CO, HDO, and H_2O but also temperature (surface and atmosphere), emissivity (if over land), and a spectrally varying gray body cloud (e.g. Kulawik *et al.,* 2006, Eldering *et al.,* 2008). As in Worden *et al*. (2006) and Worden *et al*. (2012) the constraint matrix used to regularize the HDO and H_2O components of the retrieval includes off-diagonal components that reflect *a priori* knowledge about the variability of HDO with respect to H_2O in order to ensure that the ratio of HDO to H_2O is optimized, as opposed to either HDO or H_2O alone. The prior information used for this covariance is derived from monthly climatologies using the NCAR Global Climate Model as discussed in Worden *et al*. (2006). The *a priori* profile used for the HDO/H_2O ratio is set to be constant over the whole globe, and represents the mean tropical *a priori* profile from the NCAR model. However, the H_2O *a priori* profile is allowed to vary by latitude and is based on re-analysis (Worden *et al*. 2006); therefore the HDO profile is the mean tropical profile of the HDO/H_2O ratio from the NCAR model multiplied by the H_2O *a priori* profile.

We use single pixel radiances that have not been transformed through "cloud clearing" in order to preserve the original, well characterized radiance noise characteristics for use in our estimates (Irion *et al*. 2018; DeSouza-Machado *et al*. 2018) and because we find that single-pixel AIRS radiances have sufficient information about cloud pressure and optical depth to be retrieved jointly with the trace gases, as demonstrated empirically through validation of these AIRS-based composition retrievals with TES retrievals (e.g. Figures 1 - 4) A primary difference between the retrieval approach shown in this paper versus the TES methane and HDO retrievals (Worden *et al.,* 2012) and those from previous efforts using AIRS radiances (e.g. Xiong *et al.,*

2008) is that we retrieve these trace gas profiles using the AIRS radiances from ~8 and ~12 microns instead of radiances from the 8 micron region alone. The 8 micron region used (~1217 to 1315 cm^{-1}) for these retrievals has the most sensitivity to HDO and H_2O whereas the 12 micron band (~650 to 900 cm^{-1}) is primarily sensitive to temperature and H_2O. All channels are used within this spectra unless flagged as poor during calibration. All channels are used within this spectral range unless flagged as poor during calibration. Adding the AIRS measured radiance at 12 microns is critical for reducing uncertainties in the CH_4 estimate, which is discussed in a subsequent paper.

5) Characterization of HDO/H_2O profiles

While H_2O is quantified using radiances from both the 12 micron and 8 micron spectral regions, the primary absorption lines used here to quantify HDO are in the 8 micron region. There are other HDO (and H_2O^{18}) lines available to use from the AIRS radiance but for now we only use the 8 micron region to ensure consistency between AIRS and TES data. Figure 1 shows the 8 micron radiance (top panel) and the column (log) Jacobians for H_2O and HDO respectively (middle and bottom panels) with both the H_2O and HDO Jacobians indicating sufficient sensitivity above the noise level of the radiances to variations of better than 2% in H_2O and HDO, because most values are approximately -50 or better.

Figure 2 shows the averaging kernel matrix for the HDO component of the joint retrieval. The averaging kernel describes the partial derivative of the estimate, or log(HDO), relative to its true state; consequently it can also be used to evaluate the vertical resolution and sensitivity of the estimate. For example, if the HDO/H_2O ratio varies by 100% at 908 hPa, then the AIRS estimate would be able to observe about 30% of the variability because the averaging kernel is approximately 0.3 at that level. In addition, the averaging kernel at 908 hPa depends on the deuterium content at several other pressure levels below and above, indicating that the estimate at 908 hPa also depends on the deuterium content variations at these other levels. As discussed in Worden *et al*. (2012) and Schneider *et al*. (2012), the sensitivity of the estimated HDO/H_2O ratio is limited by the sensitivity of the estimate to HDO.

Figure 3 (top panel) shows the tropospheric deuterium content (or HDO/H_2O ratio) derived from AIRS observations on July 1 2006. Despite the increased computational performance of the OSS radiative transfer calculation relative to the TES algorithm line-by-line calculation (Clough *et al*. 2005), the retrieval is still sufficiently expensive such that we only process a sub-set of the AIRS retrievals. Considering the computational cost, for the purpose of constructing a record we currently only process AIRS retrievals from between 45 S to 65 N that coincide with the nearest TES observation but with an additional two observations within 100 km of the TES track over the continents; this ad hoc sampling strategy is based on experience with previous studies using the TES deuterium and methane measurements. The traditional notation for this quantity is called "delta-D" with units of "per mil" or parts per thousand relative to the Standard Mean Ocean Water (SMOW) deuterium content which is 3.11×10^{-4} molecules of HDO per molecule of H_2O. The observations shown represent the deuterium content for the pressures between 750 hPa and 350 hPa, where we find the AIRS and TES observations have maximal overlap in their vertical resolution. The total error (middle panel) is given in units of per mil and ranges between 25 to 30 per mil. The DOFS, or trace of the averaging kernel, are shown in the bottom panel and indicate that the HDO/H_2O retrieval can resolve different parts of the troposphere, at least in the tropics, because (as demonstrated in Figure 2) the rows of the averaging kernels are separated between the boundary layer region (surface to ~750 hPa) and the free-troposphere (~600 to 300 hPa). However, these observations cannot completely resolve the total variability in these two regions of the atmosphere because the total DOFS is approximately 1.5 and for the measurement to be able to resolve the variability (to within the calculated error) of the two regions there would need to be at least 2 DOFS.

6) Comparison of AIRS and TES HDO/H_2O retrievals

Figure 4 shows a comparison between overlapping AIRS and TES estimates of the HDO/H_2O ratio for June 1 2006. The AIRS and TES measurements effectively overlap in space and within a few seconds in time as the instruments are in the same orbit. However not all the comparisons shown in Figure 4 overlap as retrievals may be rejected due to poor quality. We therefore compare all data that are within 200 km in the free troposphere. All comparisons occur during the same day with both AIRS and TES measurement taken less than a minute from each other. We do not expect substantive error to occur due to spatial mismatch of 2 degrees or less because air parcels in the free-troposphere have length scales that are several hundred kilometers long (e.g. Worden *et al*. 2013). The average between approximately 750 hPa and 350 hPa are shown for when the DOFS are larger than one for this altitude region. There is a slight bias of -2.7 +/- 1.5 per mil between TES and AIRS as shown in the top panel. The calculated and actual (RMS difference between AIRS and TES) uncertainties are shown and are approximately 30 per mil, primarily driven by the uncertainty in the AIRS based estimates as the TES based estimates have an uncertainty of approximately 15 per mil. The errors are calculated during the optimal estimation retrieval (Bowman *et al*. 2007; Worden *et al*. 2012) and depend on the expected noise of the AIRS radiances and the parameters that are co-retrieved with the AIRS HDO/H_2O ratio such as temperature, surface emissivity, clouds, and methane. As noted in Worden *et al*. (2012) these co-retrieved parameters affect both the precision and accuracy whereas the noise only affects the precision.

A comparison of the AIRS and TES HDO/H_2O ratio for five single global surveys taken between 2006 and 2010 (one global survey per year during boreal summer) is shown in Table 1 and indicate that the overall bias varies between -2.7 to 3.7 per mil, for these comparisons. Using all 5 TES global surveys that are summarized in Table 1 we can construct how AIRS and TES compare as a function of latitude as shown in Figure 5. Figure 5 is constructed by averaging the difference between TES and AIRS observations within 5 degree latitudinal bins. The mean bias across latitudes is ~-2.6 per mil. The error shown on the difference is the error on the mean, which is the Root-Mean-Square (RMS) of the differences divided by the square root of the number of co-located observations. The RMS of the latitudinal variability is ~7.8 per mil which is similar to the mean variations shown in Table 1 and also the accuracy of the Aura TES delta-d observations that are based on comparisons of TES data with surface and aircraft measurements (Worden *et al*. 2011; Herman *et al*. 2014). We therefore take the accuracy of the AIRS data to be ~7.8 per mil. These comparisons therefore show that the AIRS estimates of the HDO/H_2O ratio are robust as the calculated and actual uncertainties are consistent with an accuracy comparable to observations from TES.

8) Conclusion

This paper describes the vertical resolution and error characteristics of retrievals of the deuterium content (HDO and H_2O) of water vapor using AIRS radiances and then evaluates the consistency between AIRS and TES retrievals of HDO and H_2O. We find that the AIRS and TES deuterium content for the lower-troposphere (750 – 350 hPa) are consistent, or within their calculated uncertainties, for the 5 year period in which TES observations span the globe (2006-2010). We find the total uncertainty for a single AIRS observation is ~30 per mil with an accuracy of ~7.8 per mil. These uncertainties can be compared to the total variability, which can range from -300 to 0 per mil over the whole globe.

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Table 1: Comparison between averaged TES and AIRS HDO/H_2O ratio (750-350 hPa). The units are in parts per thousand relative to Standard Mean Ocean Water. The last row shows the average and RMS for the mean differences in the far right column.

Date	Expected RMS (per mil / SMOW)	Actual RMS (per mil / SMOW)	Mean (TES-AIRS) (per mil / SMOW)
2006-06-01	31.1	30.6	-2.7 +/- 1.5
2007-06-02	30.0	31.9	-0.6 +/- 1.5
2008-06-02	31.5	29.3	0.5 +/- 1.4
2009-07-06	31.6	27.1	0.7 +/- 1.4
2010-06-02	31.6	28.2	3.7 +/- 1.2

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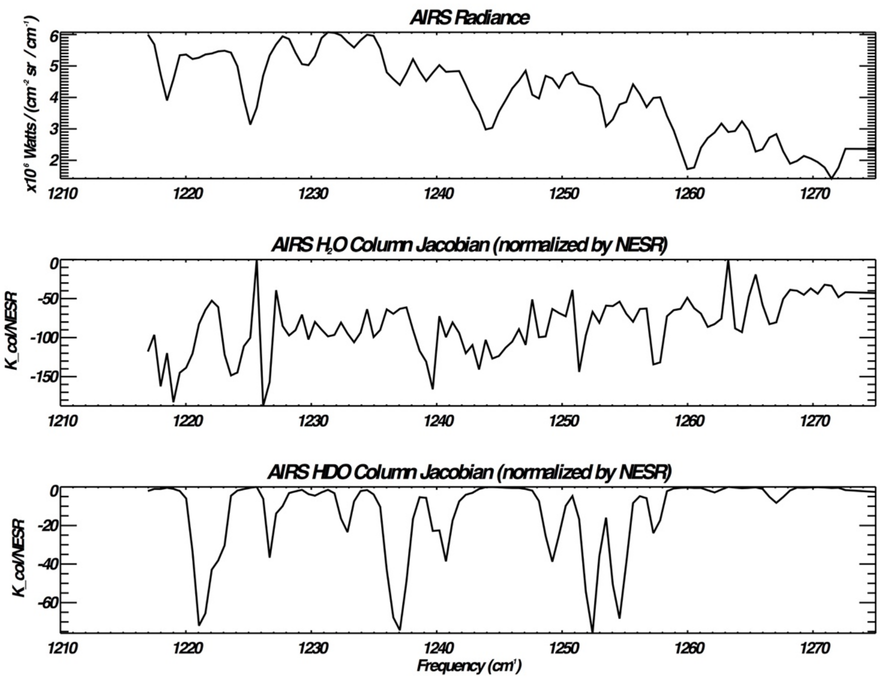

Figure 1: (top) AIRS radiance at approximately 8 microns for a typical tropical scene. (middle) The total column (log) Jacobian for H_2O normalized by the AIRS NESR. (bottom) The total column (log) Jacobian for HDO normalized by the AIRS NESR.

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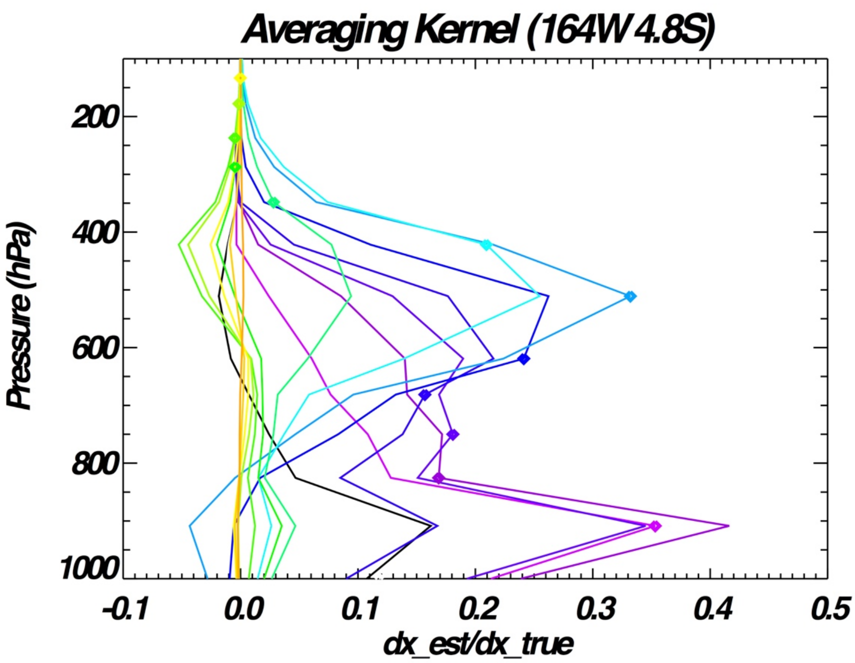

Figure 2: The rows of the averaging kernel matrix for the HDO retrieval corresponding to the radiance shown in Figure 1. The different colors and symbols are to indicate the pressure levels corresponding to each row of the averaging kernel matrix.

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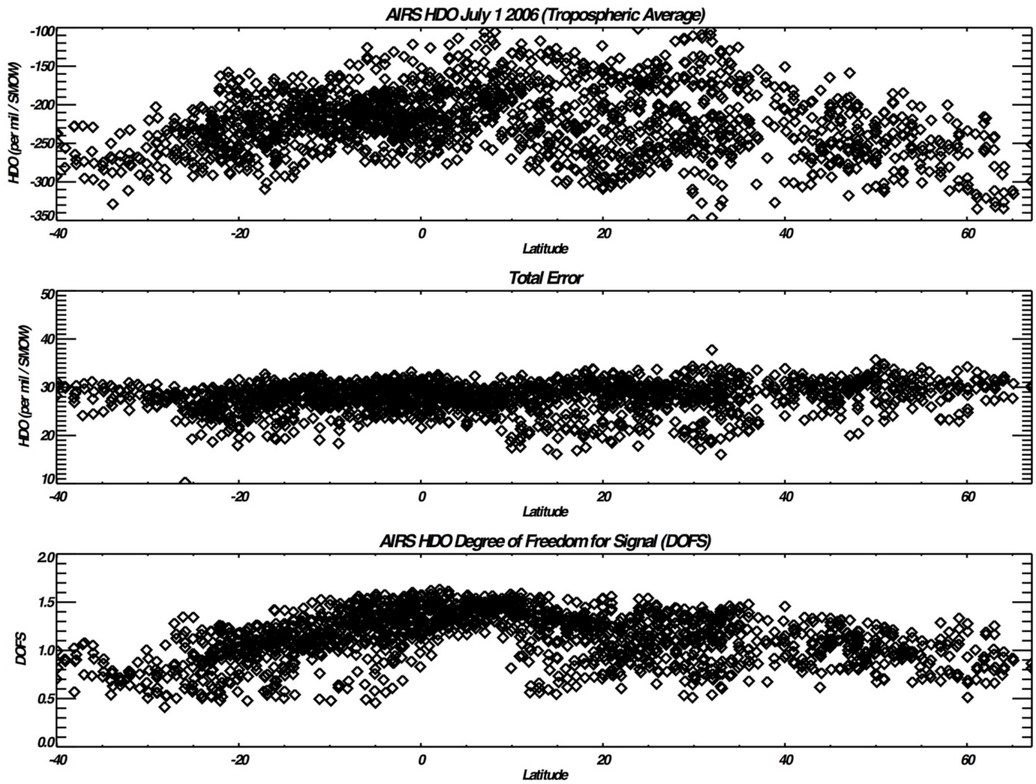

Figure 3: (top) The mean tropospheric deuterium content (in “per mil” or units of parts per thousand relative to the deuterium content of the ocean or SMOW) for June 1 2006 as inferred from AIRS radiance measurements. (middle) The total error for the measurements in the top panel (also in units of per mil relative to SMOW). (bottom) The DOFS for the retrieval.

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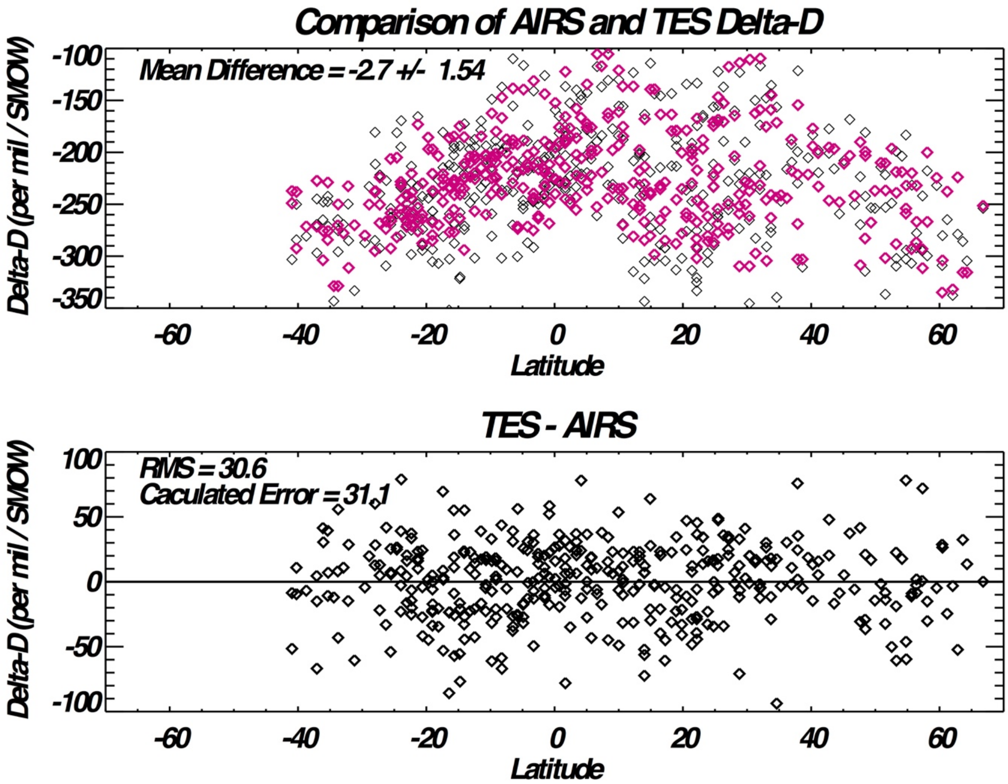

Figure 4: (top) Comparison of AIRS and TES delta-d for June 1 2006 (~600 co-located observations) . (bottom) the differences (after bias subtraction) between TES and AIRS.

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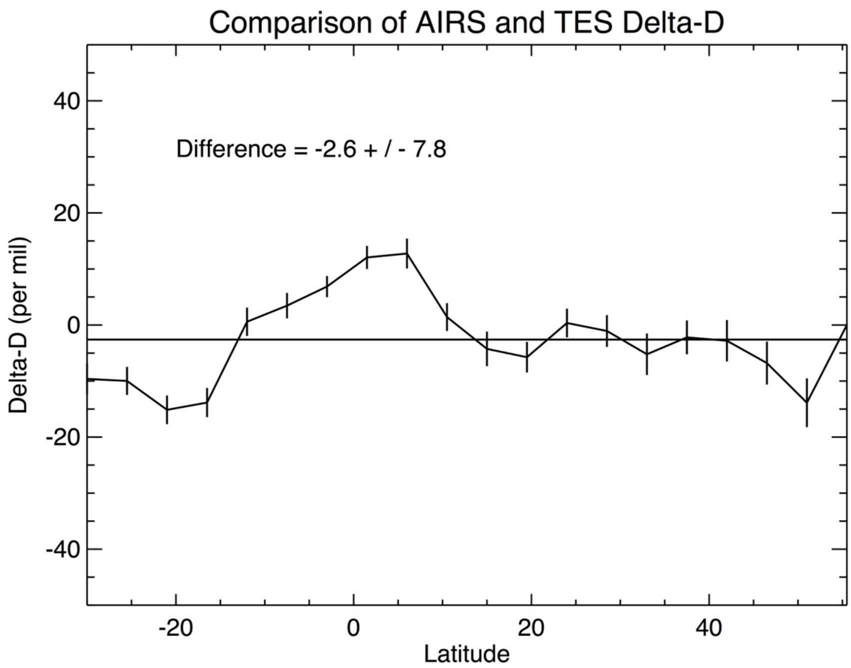

Figure 5: Comparison of the Latitudinal differences between TES and AIRS Delta-D using co-located observations for 5 days (approximately 600 observations per day) of data, spaced over 5 N. Hemisphere summers between 2006 and 2010.