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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. We evaluate the error characteristics and vertical sensitivity of AIRS measurements corresponding to five days of TES data (or 5 global surveys) during the Northern 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 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 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, as compared to ~15 per mil for the TES data. Comparison with the TES data also indicate that the uncertainty of a single target AIRS HDO/H_2O measurement is ~30 per mil. Comparison of AIRS and TES data between 30 degrees South and 50 degrees North indicate 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.

Introduction:

Measurements of the isotopic composition of water can help identify the source of the water and provide knowledge about its condensation and evaporation history (e.g. Galewsky *et al*. and refs therein). Through most of the twentieth century, most isotopic measurements of water have been of precipitation (e.g. Craig, 1961). Near global measurements of the isotopic composition of water vapor became possible with the advent of spectroscopic techniques applied to in situ measurements (e.g., Noone *et al*., 2011) using lasers and for passive ground based and satellite measurements (e.g. Worden *et al*., 2006; Frankenberg *et al*. 2009; Schneider *et al*. 2012; Lacour *et al*. 2012). These data have in turn been used to evaluate the role of convection, large scale dynamics, and evapotranspiration on the tropical water cycle (e.g. Worden *et al*. 2007; Frankenberg *et al*. 2009; Wright *et al*. 2017) tropical convection (e.g. Lacour 2018 and refs therein) and the role of plants on global evapotranspiration (Good *et al*. 2015).

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 measurements. Our goal is to create a multi-decadal Earth Science Data Record (ESDR) using the AIRS and TES data; the TES global record spans ~6 years (2005-2010) and the AIRS data span 17+ years starting in 2002. This ESDR could potentially be used for evaluating the changing water cycle (e.g. Bailey *et al.,* 2017) and its coupling to the carbon cycle (e.g. Zhou *et al.,* 2014; Wright *et al.,* 2017).

We first characterize the vertical resolution and uncertainties for estimates of HDO and H_2O, and their ratio, using AIRS radiance observations corresponding to boreal 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 measurements remained the same. We make only these comparisons due to current processing limitations but expect additional overlap between TES and AIRS data sets in the coming years. We then compare the AIRS and TES data to evaluate the calculated uncertainties of the AIRS data.

1) 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}; 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; with the ~1650 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 Aura TES instrument 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 also 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 ESDR's.

3) Description of the 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 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 the version 4 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 the Retrieval Approach

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; however, we will briefly 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 geophysical observables that affect the corresponding radiance.

For the AIRS retrievals discussed here, 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 retrieval of 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). We assume the noise in any given pixel is uncorrelated with those from adjacent pixels. However, these correlations are known to exist (e.g. Pagano *et al*. 2008) and the impact of ignoring them is that our calculated uncertainties will be larger than expected and therefore our noise related uncertainty should be considered a conservative estimate.

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 in order to provide a stronger constraint on atmospheric temperature and hence reduce uncertainty from knowledge of temperature on the HDO and H_2O retrieval. 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.

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) 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 Jacobian, or sensitivity of the radiance to variations in the (log) H_2O and (log) HDO respectively (middle and bottom panels). These Jacobians are normalized by the instrument noise. For example, a value of 1 means that it would take a 100% change in the corresponding species to distinguish between two similar radiances (everything about the observed scene and radiance is the same except for the species of interest) above the noise level. A value of ~-50 therefore means that only a 2% variation is required (or 1/50).

Figure 2 shows the averaging kernel matrix for the HDO component of the joint retrieval. The averaging kernel describes the response of the estimate, or log(HDO), relative to variations in the true state; consequently it can also be used to evaluate the vertical resolution and sensitivity of the estimate. For example, if HDO 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. The averaging kernel at 908 hPa also depends on the deuterium content at several other pressure levels below and above indicating that the estimate at 908 hPa depends on the deuterium content variations at these other levels. Not shown are the dependencies of the (log) HDO estimate to those from the (log) H_2O estimate. These dependencies between the HDO averaging kernels and with the H_2O averaging kernels are accounted for when constructing the HDO/H_2O ratio; however a residual uncertainty called the "smoothing" error is imparted when comparing the HDO/H_2O ratio to independent data; this smoothing error is part of the error budget shown in Figure 3. 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. Users of these data should note that this ratio is typically used with that of H_2O in order to better evaluate their joint variation (HDO/H_2O, H_2O) against simple mixing and rainfall models (Noone *et al.* 2011). However, the sensitivity of the radiance to H_2O variations is much stronger than that for HDO, although the altitude region of the HDO sensitivity typically overlaps with the H_2O sensitivity. Schneider *et al.* (2012) discusses how to created HDO/H_2O, H_2O pairs to mitigate this component of the smoothing error when comparing these data against the simple models described in Noone *et al.* (2011). For comparison to more complex global climate models the user of these data also needs to apply the HDO and H_2O averaging kernels to the corresponding model fields (e.g. Risi *et al.*, 2012).

Figure 3 (top panel) shows the tropospheric deuterium content (or HDO/H_2O ratio) derived from AIRS observations on July 1 2006. Despite the improved 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 can 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 degrees South to 65 degrees North 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" , or "δ-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 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. 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 many of the HDO/H_2O retrievals 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 typically 1.5 or less 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. 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. Figure 5 shows a direct comparison of the AIRS and TES data. The correlation is about 0.89 and the one-to-one line (solid line) overlaps this distribution. However the lowest values likely diverge from the one-to-one line, possibly because the vertical distribution in the sensitivity depends on the amount of HDO and hence we should expect differences between the TES and AIRS deuterium measurements for these lower-sensitivity retrievals.

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 indicates that the overall bias varies between -2.7 to 3.7 per mil. 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 6. Figure 6 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 bars 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; as this error bar is a measure of precision for each latitude bin, this comparison demonstrates that there are variations in the comparison that are larger than the precision and are therefore related to systematic errors in either the TES data or AIRS data or both. Variations in these systematic errors can be seen in the latitudinal variability, which has an RMS variation of ~7.8 per mil for the different latitude bins but can vary by as much as ~-15 to ~+15 per mil in the tropics. Typically these variations are due to a combination of uncertainties in the spectroscopy along with temperature, water vapor, and surface properties; they may also be due to "smoothing error" which is related to how differences in the vertical resolution affect the tropospheric average of the deuterium content shown in these figures (e.g. Worden *et al*. 2004). This 7.8 per mil variation across latitudes is about the same as the reported 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 report the current accuracy of the AIRS data to be ~7.8 per mil. We expect future comparisons between these data and those from aircraft or revisions to the AIRS retrieval approach will modify this estimate of the accuracy.

8) Conclusion

This paper describes the vertical resolution and error characteristics of retrievals of the deuterium content (or the HDO/H_2O ratio) 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 observed total variability, which can range from approximately -350 to -50 per mil over the whole globe, as observed by the Aura TES data (Worden *et al*. 2006) and shown in Figure 3 for AIRS data.

While only five days of comparisons are shown here for the purpose of evaluating the retrieval approach and error characteristics of these AIRS retrievals, we expect to produce a record of the AIRS-based deuterium content retrievals from the start of the mission (2002) through the present. Because of computational limitations, we expect to process data from 45 degrees South to 65 degrees North at approximately four times the sampling of the Aura TES measurements and with increased sampling (~3x) over the continental regions with the goal of increasing this sampling once the initial record is completed and as additional resources become available.

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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 second column shows the expected RMS based on the uncertainties of the TES and AIRS data. The third column shows the actual RMS difference between TES and AIRS. The last column shows the mean difference.

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

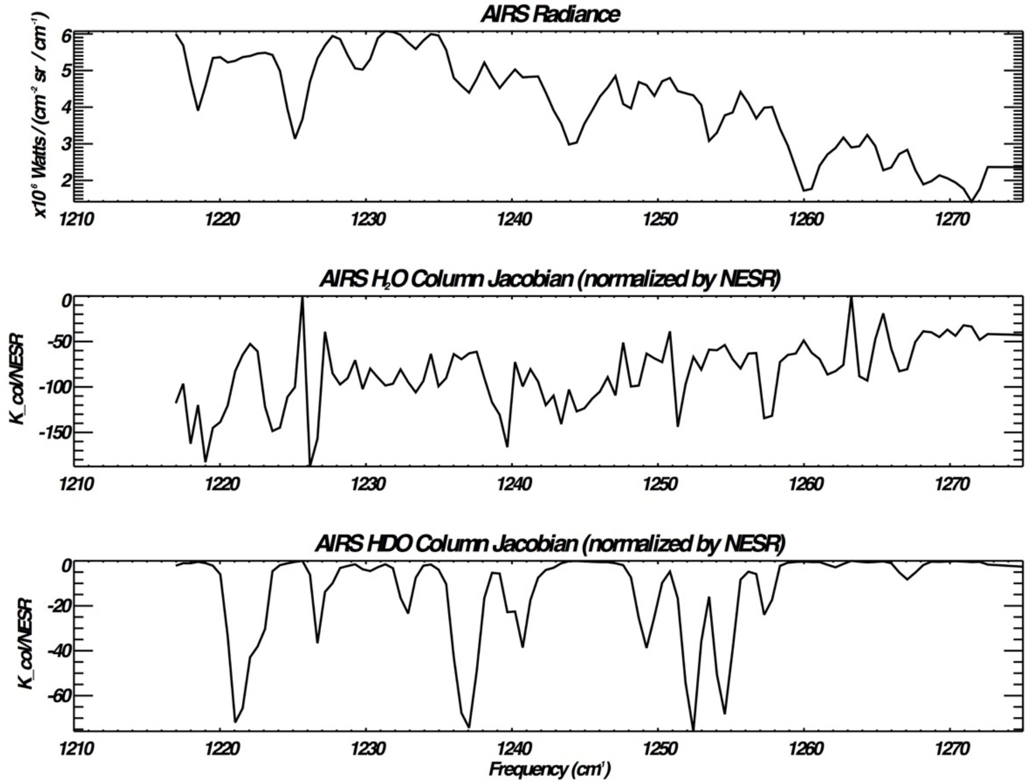

Figure 1: (top) AIRS radiance at approximately 8 microns for a typical tropical scene. (middle) The total column (log) Jacobian for H_2O normalized by the AIRS NESR. (bottom) The total column (log) Jacobian for HDO normalized by the AIRS NESR.

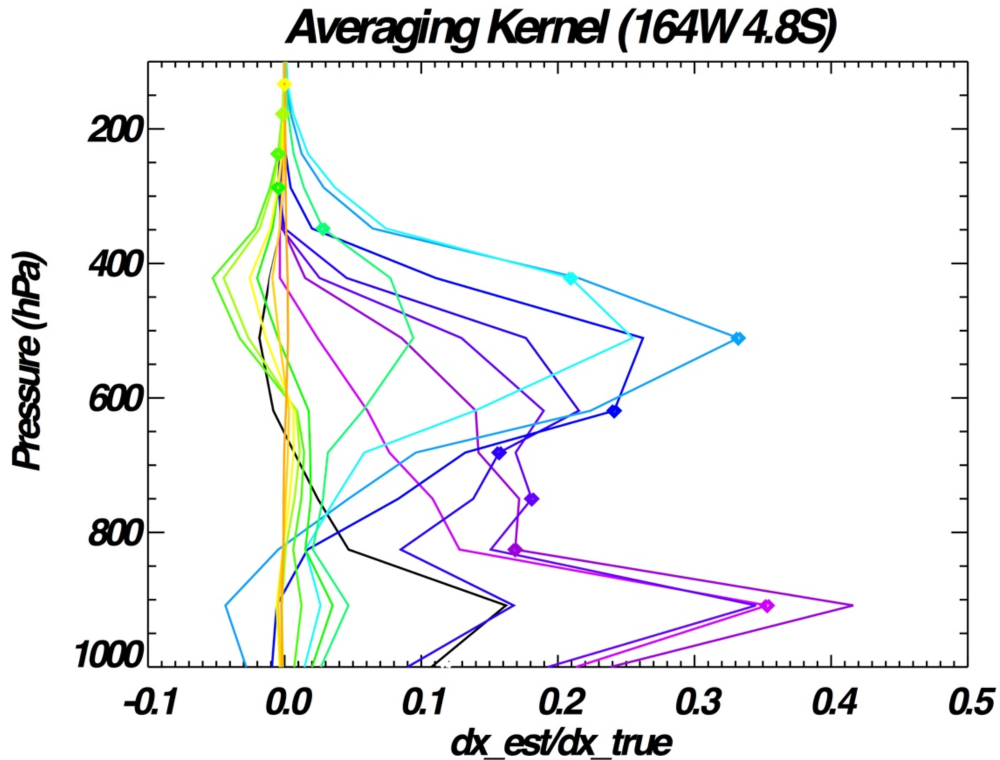

Figure 2: The rows of the averaging kernel matrix for the HDO retrieval corresponding to the radiance shown in Figure 1. The different colors and symbols are used to indicate the pressure levels corresponding to each row of the averaging kernel matrix.

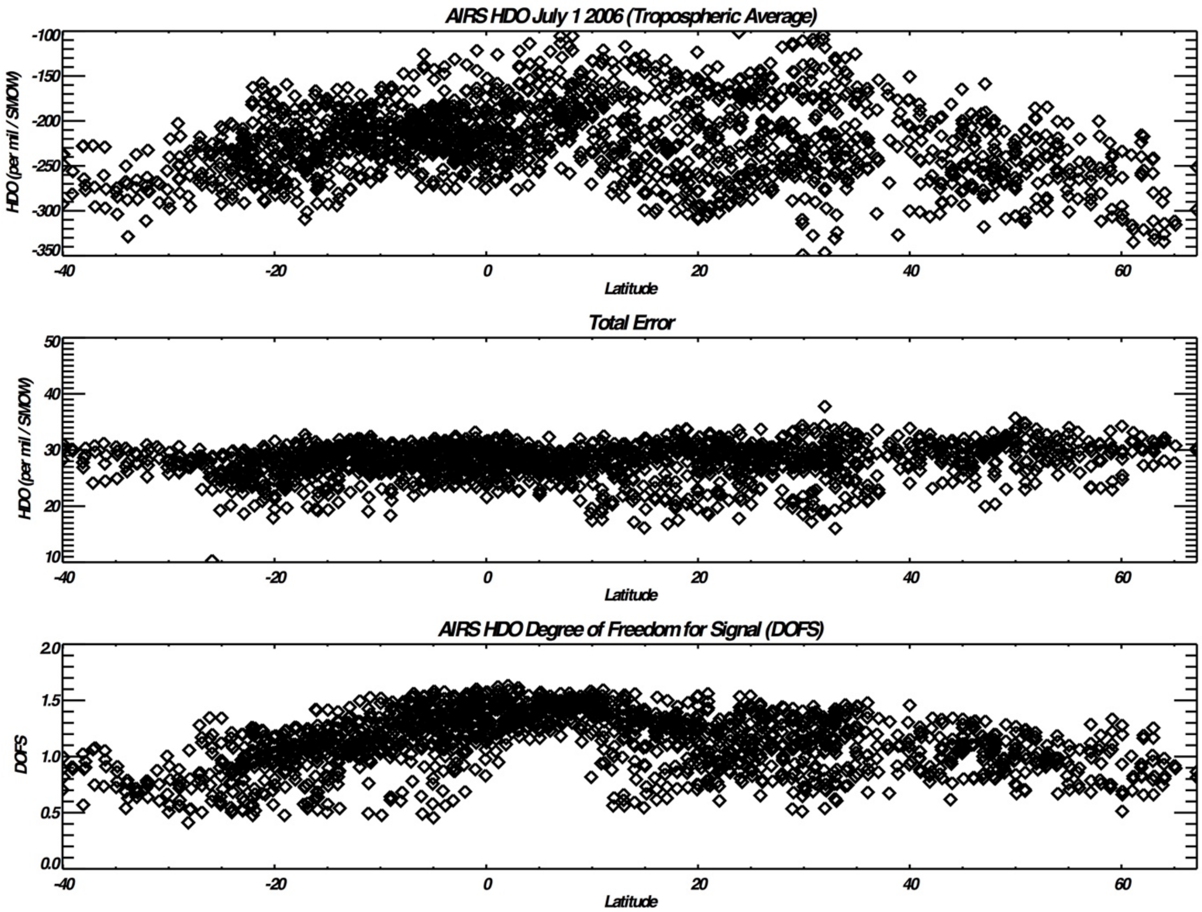

Figure 3: (top) The mean tropospheric deuterium content (in "per mil" or units of parts per thousand relative to the deuterium content of the ocean or SMOW) for June 1 2006 as inferred from AIRS radiance measurements. (middle) The total error for the measurements in the top panel (also in units of per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

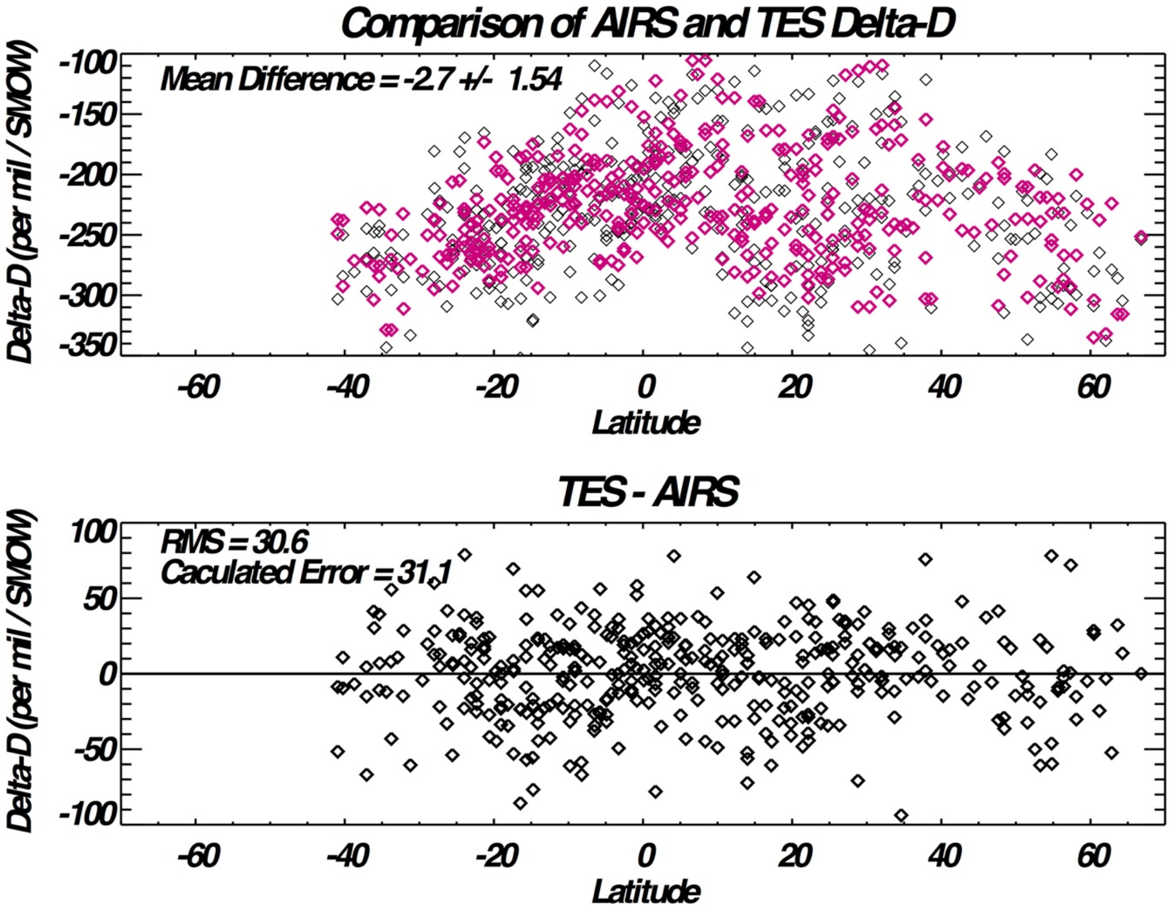

Figure 4: (top) Comparison of AIRS (red) and TES (black) delta-D for June 1 2006 (~600 co-located observations). (bottom) The differences (after bias subtraction) between TES and AIRS delta-D measurements.

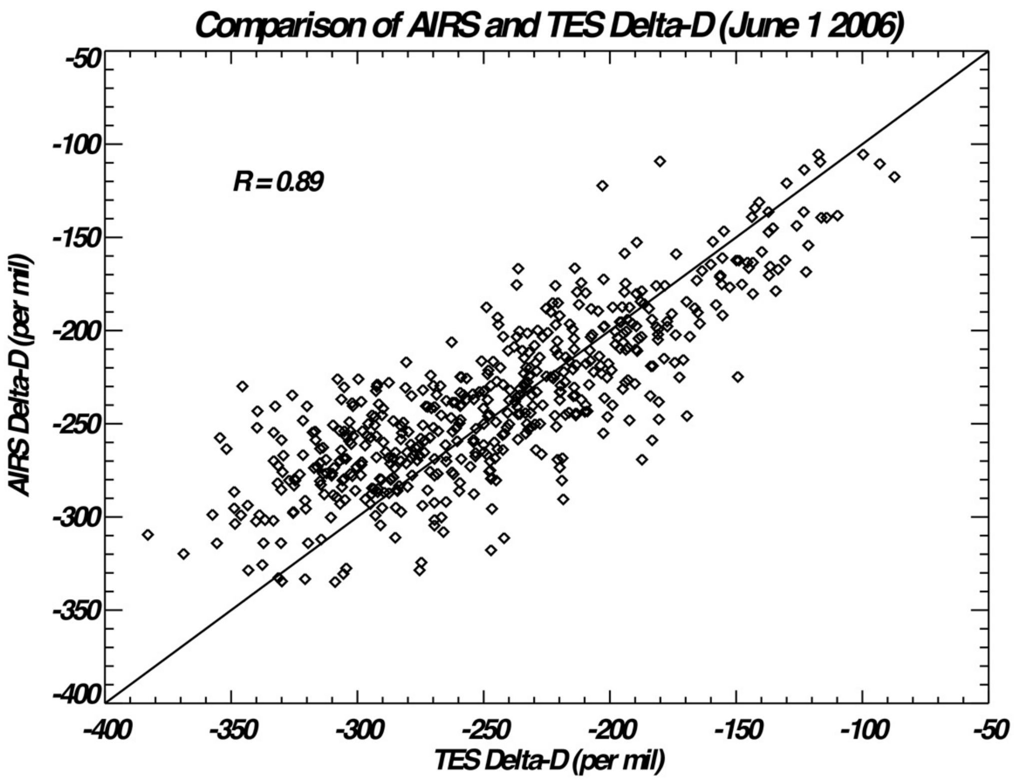

Figure 5: Comparison of the AIRS and TES deuterium content. The solid line is the one-to-one line.

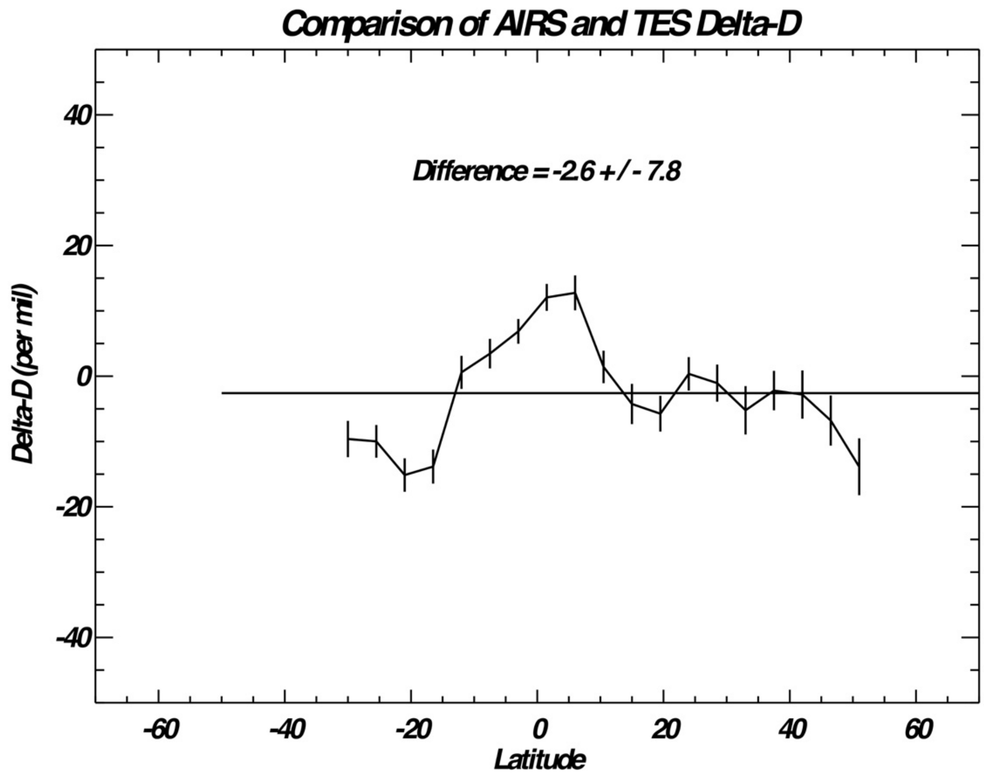

Figure 6: The Latitudinal differences between TES and AIRS Delta-D using co-located observations for 5 days (approximately 600 observations per day) of data, spaced over 5 Northern Hemisphere summers between 2006 and 2010.