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

11  
12 **Abstract:** Single pixel, tropospheric retrievals of HDO and H<sub>2</sub>O concentrations are retrieved  
13 from Atmospheric Infrared Sounder (AIRS) radiances using the optimal estimation algorithm  
14 developed for the Aura Tropospheric Emission Spectrometer (TES) project. We evaluate the  
15 error characteristics and vertical sensitivity of AIRS measurements corresponding to five days of  
16 TES data (or 5 global surveys) during the Northern Hemisphere summers between 2006 and  
17 2010 (~600 co-located comparisons per day). We find that the retrieval characteristics of the  
18 AIRS deuterium content measurements have similar vertical resolution middle-troposphere as  
19 TES but with slightly less sensitivity in the lower-most troposphere, with a typical degrees-of-  
20 freedom (DOFS) in the tropics of 1.5 and approximately double the uncertainty. The calculated  
21 measurement uncertainty is ~30 per mil (parts per thousand relative to the deuterium  
22 composition of ocean water) for a tropospheric average between 750 and 350 hPa, the altitude  
23 region where AIRS is most sensitive. Comparison with the TES data also indicate that the  
24 uncertainty of a single target AIRS HDO/H<sub>2</sub>O measurement is ~30 per mil. Comparison of AIRS  
25 and TES data between 30 degrees South and 50 degrees North indicate that the AIRS data is  
26 biased low by ~2.6 per mil with a latitudinal variation of ~7.8 per mil. This latitudinal variation  
27 is consistent with the accuracy of TES data as compared to in situ measurements, suggesting that  
28 both AIRS and TES have similar accuracy.

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TES observations taken between 2006 through 2010.

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1 **Introduction:**

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

13 In this paper we demonstrate a retrieval algorithm, based upon the Aura TES optimal  
14 estimation retrieval algorithm (e.g. Worden et al. 2012) that can provide robustly characterized  
15 measurements of the deuterium content of water vapor (HDO and H<sub>2</sub>O) from the AIRS  
16 measurements. Our goal is to create a multi-decadal Earth Science Data Record (ESDR), using  
17 the AIRS and TES data; the TES global record spans ~6 years (2005-2010) and the AIRS data  
18 span 17+ years starting in 2002. This ESDR could potentially be used for evaluating the  
19 changing water cycle (e.g. Bailey et al., 2017) and its coupling to the carbon cycle (e.g. Zhou et  
20 al., 2014; Wright et al., 2017).

21 We first characterize the vertical resolution and uncertainties for estimates of HDO and  
22 H<sub>2</sub>O, and their ratio, using AIRS radiance observations corresponding to boreal summertime TES  
23 global survey's between 2006 through 2010, which is the time period when TES observations  
24 sample the (near) global atmosphere and the calibration approach for TES measurements  
25 remained the same. We make only these comparisons due to current processing limitations but  
26 expect additional overlap between TES and AIRS data sets in the coming years. We then  
27 compare the AIRS and TES data to evaluate the calculated uncertainties of the AIRS data.

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29 **1) Description of AIRS and TES instruments**  
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31 The AIRS instrument is a nadir-viewing, scanning infrared spectrometer (Aumann et al.  
32 2003; Pagano et al., 2003; Irion et al. 2018; DeSouza-Machado et al. 2018) that is onboard the

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- Deleted: 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<sub>4</sub> 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.
- Deleted: H<sub>2</sub>O
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- Deleted: 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.
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1 NASA Aqua satellite and was launched in 2002. AIRS measures the thermal radiance between  
2 approximately 3-12 microns with a resolving power of approximately 1200. For the 8 micron  
3 spectral range used for the HDO/H<sub>2</sub>O retrievals, the spectral resolution is ~1 cm<sup>-1</sup> with a gridding  
4 of ~0.5 cm<sup>-1</sup>; the signal-to-noise (SNR) ranges from ~400 to ~1000 over the 8 micron region for a  
5 typical tropical scene. A single footprint has a diameter of ~15 km in the nadir; with the ~1650  
6 km swath, the AIRS instrument can measure nearly the whole globe in a single day. The Aqua  
7 satellite is part of the “A-Train” that consists of multiple satellites, including TES, in a sun-  
8 synchronous orbit at 705 km with an approximately 1:30 pm equator crossing-time.

9 The Aura TES instrument is a Fourier Transform Spectrometer that originally was  
10 designed to measure the thermal infrared (IR) radiances both in the limb and nadir viewing in  
11 order to obtain vertically resolved trace gas profiles of ozone, CO, CH<sub>4</sub>, HDO and H<sub>2</sub>O, and  
12 several ozone pre-cursors such as ammonia, methanol, and PAN (e.g. Beer *et al.*, 2001; Worden  
13 *et al.*, 2004; Worden *et al.* 2006; Luo *et al.*, 2007; Beer *et al.* 2008; Worden *et al.*, 2012; Payne *et*  
14 *al.* 2014). Several of these trace gases, such as CO, CH<sub>4</sub>, and ammonia have also been quantified  
15 using AIRS radiances (e.g. McMillan *et al.*, 2005; Xiong *et al.* 2008; Warner *et al.*, 2016). In  
16 comparison to the AIRS instrument, TES has a spectral resolution of ~0.12 cm<sup>-1</sup> (apodized) with  
17 a spectral gridding of 0.06 cm<sup>-1</sup>. The SNR is ~300 in the 8 microns spectral region. The Aura TES  
18 instrument, after the summer of 2005, observes one nadir scene every 100 km along the orbit  
19 path. The effective length of the record is approximately five years, between September 2005  
20 through November 2009, after which instrument degradation problems resulted in interrupts and  
21 a decrease in sampling. The AIRS instrument has nearly one thousand times the sampling of TES  
22 and near continuous operation between 2002 through the present and therefore can be used to  
23 construct several composition based ESDR's,

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### 25 3) Description of the Radiative Transfer Forward Model

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

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1 specific frequency range and spectral resolution to increase the radiative transfer calculation  
2 performance by approximately a factor of 20-100 relative to a line-by-line calculation  
3 (<http://rtweb.aer.com> ). OSS can be trained to user-defined accuracy relative to the line-by-line  
4 model used for training. Here, the training threshold was set to 20 % of the AIRS noise level.  
5 The line-by-line model used as a reference in the training and to build the absorption coefficient  
6 look-up tables (LUTs) used by the fast RTM is the Line-By-Line Radiative Transfer Model  
7 (LBLRTM) (Clough et al., 2005; Alvarado et al., 2013). The OSS version used in this work is  
8 based on LBLRTM v12.4, using the TES\_v2.0 spectroscopic line parameter database. The  
9 TES\_v2.0 line parameter database follows the HITRAN 2012 compilation (Rothman et al.,  
10 2013)], with the following exceptions:

- 11 • H<sub>2</sub>O positions and intensities are taken from the aer\_v\_3.4 line parameter database  
12 (<http://rtweb.aer.com>), closely following the measured and calculated values published in  
13 Coudert et al. (2008).
- 14 • CH<sub>4</sub> includes first order line mixing coefficients (as supplied in the aer\_v\_3.4 line  
15 parameter database). These were calculated using the approach of Tran et al. (2006).
- 16 • CO<sub>2</sub> line parameters are from the database of Lamouroux et al. (2015). This database  
17 takes most of its line positions, intensities, and lower state energies from the HITRAN  
18 2012 database, but the values for air-broadening half-widths and their temperature  
19 dependences are adjusted from the HITRAN 2012 values to be consistent  
20 throughout the bands, and the air-induced pressure shifts (not given for a majority of  
21 transitions in HITRAN 2012) were added. The TES\_v2.0 database includes first order  
22 line mixing coefficients (as supplied in the aer\_v\_3.4.1 line parameter database),  
23 calculated using the software of Lamouroux et al. (2015).

24 Further information on the AER line parameter databases can be found at <http://rtweb.aer.com>.  
25 OSS is adapted for use with AIRS radiances using the version 4 AIRS spectral response function  
26 (SRF) (Strow et al., 2003) that is interpolated to a uniform grid of 0.004 cm<sup>-1</sup> centered on the  
27 channel center frequencies. The OSS radiative transfer code provides speedup of 20-100x over  
28 the original TES operational radiation transfer model (Clough *et al.*, 2006).

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#### 30 4) Description of the Retrieval Approach

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The optimal estimation algorithm used in this analysis for quantifying CH<sub>4</sub>, HDO, H<sub>2</sub>O, 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<sub>4</sub>, CO, HDO, and H<sub>2</sub>O 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<sub>2</sub>O components of the retrieval includes off-diagonal components that reflect *a priori* knowledge about the variability of HDO with respect to H<sub>2</sub>O in order to ensure that ~~retrieval of~~ the ratio of HDO to H<sub>2</sub>O is optimized, as opposed to either HDO or H<sub>2</sub>O 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<sub>2</sub>O 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<sub>2</sub>O 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<sub>2</sub>O ratio from the NCAR model multiplied by the H<sub>2</sub>O 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~~

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1 are known to exist (e.g. Pagano *et al.* 2008) and the impact of ignoring them is that our  
2 calculated uncertainties will be larger than expected and therefore our noise related uncertainty  
3 should be considered a conservative estimate.

4 A primary difference between the retrieval approach shown in this paper versus the TES  
5 methane and HDO retrievals (Worden *et al.*, 2012) and those from previous efforts using AIRS  
6 radiances (e.g. Xiong *et al.*, 2008) is that we retrieve these trace gas profiles using the AIRS  
7 radiances from ~8 and ~12 microns instead of radiances from the 8 micron region alone in order  
8 to provide a stronger constraint on atmospheric temperature and hence reduce uncertainty from  
9 knowledge of temperature on the HDO and H<sub>2</sub>O retrieval. The 8 micron region used (~1217 to  
10 1315 cm<sup>-1</sup>) for these retrievals has the most sensitivity to HDO and H<sub>2</sub>O whereas the 12 micron  
11 band (~650 to 900 cm<sup>-1</sup>) is primarily sensitive to temperature and H<sub>2</sub>O. All channels are used  
12 within this spectra unless flagged as poor during calibration.

### 14 5) Characterization of HDO/H<sub>2</sub>O profiles

16 While H<sub>2</sub>O is quantified using radiances from both the 12 micron and 8 micron spectral  
17 regions, the primary absorption lines used here to quantify HDO are in the 8 micron region.  
18 There are other HDO (and H<sub>2</sub>O) lines available to use from the AIRS radiance but for now we  
19 only use the 8 micron region to ensure consistency between AIRS and TES data. Figure 1 shows  
20 the 8 micron radiance (top panel) and the Jacobian, or sensitivity of the radiance to variations in  
21 the (log) H<sub>2</sub>O and (log) HDO respectively (middle and bottom panels). These Jacobians are  
22 normalized by the instrument noise. For example, a value of 1 means that it would take a 100%  
23 change in the corresponding species to distinguish between two similar radiances (everything  
24 about the observed scene and radiance is the same except for the species of interest) above the  
25 noise level. A value of ~50 therefore means that only a 2% variation is required (or 1/50).

26 Figure 2 shows the averaging kernel matrix for the HDO component of the joint retrieval.  
27 The averaging kernel describes the response of the estimate, or log(HDO), relative to variations  
28 in the true state; consequently it can also be used to evaluate the vertical resolution and  
29 sensitivity of the estimate. For example, if HDO varies by 100% at 908 hPa, then the AIRS  
30 estimate would be able to observe about 30% of the variability because the averaging kernel is  
31 approximately 0.3 at that level. The averaging kernel at 908 hPa also depends on the deuterium

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1 content at several other pressure levels below and above, indicating that the estimate at 908 hPa  
2 depends on the deuterium content variations at these other levels. Not shown are the  
3 dependencies of the (log) HDO estimate to those from the (log) H<sub>2</sub>O estimate. These  
4 dependencies between the HDO averaging kernels and with the H<sub>2</sub>O averaging kernels are  
5 accounted for when constructing the HDO/H<sub>2</sub>O ratio; however a residual uncertainty called the  
6 “smoothing” error is imparted when comparing the HDO/H<sub>2</sub>O ratio to independent data; this  
7 smoothing error is part of the error budget shown in Figure 3. As discussed in Worden *et al.*  
8 (2012) and Schneider *et al.* (2012), the sensitivity of the estimated HDO/H<sub>2</sub>O ratio is limited by  
9 the sensitivity of the estimate to HDO. Users of these data should note that this ratio is typically  
10 used with that of H<sub>2</sub>O in order to better evaluate their joint variation (HDO/H<sub>2</sub>O, H<sub>2</sub>O) against  
11 simple mixing and rainfall models (Noone *et al.* 2011). However, the sensitivity of the radiance  
12 to H<sub>2</sub>O variations is much stronger than that for HDO, although the altitude region of the HDO  
13 sensitivity typically overlaps with the H<sub>2</sub>O sensitivity. Schneider *et al.* (2012) discusses how to  
14 create HDO/H<sub>2</sub>O, H<sub>2</sub>O pairs to mitigate this component of the smoothing error when comparing  
15 these data against the simple models described in Noone *et al.* (2011). For comparison to more  
16 complex global climate models the user of these data also needs to apply the HDO and H<sub>2</sub>O  
17 averaging kernels to the corresponding model fields (e.g. Risi *et al.*, 2012).  
18 Figure 3 (top panel) shows the tropospheric deuterium content (or HDO/H<sub>2</sub>O ratio)  
19 derived from AIRS observations on July 1 2006. Despite the improved computational  
20 performance of the OSS radiative transfer calculation relative to the TES algorithm line-by-line  
21 calculation (Clough *et al.* 2005), the retrieval is still sufficiently expensive such that we can only  
22 process a sub-set of the AIRS retrievals. Considering the computational cost, for the purpose of  
23 constructing a record we currently only process AIRS retrievals from between 45 degrees South  
24 to 65 degrees North that coincide with the nearest TES observation but with an additional two  
25 observations within 100 km of the TES track over the continents; this ad hoc sampling strategy is  
26 based on experience with previous studies using the TES deuterium and methane measurements.  
27 The traditional notation for this quantity is called “delta-D” , or “δ-D” with units of “per mil” or  
28 parts per thousand relative to the Standard Mean Ocean Water (SMOW) deuterium content  
29 which is  $3.11 \times 10^4$  molecules of HDO per molecule of H<sub>2</sub>O. The observations shown represent  
30 the deuterium content for the pressures between 750 hPa and 350 hPa, where we find the AIRS  
31 and TES observations have maximal overlap in their vertical resolution.

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1        The errors are calculated during the optimal estimation retrieval (Bowman *et al.* 2007;  
2 Worden *et al.* 2012) and depend on the expected noise of the AIRS radiances and the parameters  
3 that are co-retrieved with the AIRS HDO/H<sub>2</sub>O ratio such as temperature, surface emissivity,  
4 clouds, and methane. As noted in Worden *et al.* (2012) these co-retrieved parameters affect both  
5 the precision and accuracy whereas the noise only affects the precision. The total error (middle  
6 panel) is given in units of per mil and ranges between 25 to 30 per mil. The DOFS, or trace of  
7 the averaging kernel, are shown in the bottom panel and indicate that many of the HDO/H<sub>2</sub>O  
8 retrievals can resolve different parts of the troposphere, at least in the tropics, because (as  
9 demonstrated in Figure 2) the rows of the averaging kernels are separated between the boundary  
10 layer region (surface to ~750 hPa) and the free-troposphere (~600 to 300 hPa). However, these  
11 observations cannot completely resolve the total variability in these two regions of the  
12 atmosphere because the total DOFS is typically 1.5 or less and for the measurement to be able to  
13 resolve the variability (to within the calculated error) of the two regions there would need to be  
14 at least 2 DOFS.

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## 16 **6) Comparison of AIRS and TES HDO/H<sub>2</sub>O retrievals**

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18        Figure 4 shows a comparison between overlapping AIRS and TES estimates of the  
19 HDO/H<sub>2</sub>O ratio for June 1 2006. The AIRS and TES measurements effectively overlap in space  
20 and within a few seconds in time as the instruments are in the same orbit. However not all the  
21 comparisons shown in Figure 4 overlap as retrievals may be rejected due to poor quality. We  
22 therefore compare all data that are within 200 km in the free troposphere. We do not expect  
23 substantive error to occur due to spatial mismatch of 2 degrees or less because air parcels in the  
24 free-troposphere have length scales that are several hundred kilometers long (e.g. Worden *et al.*  
25 2013). The average between approximately 750 hPa and 350 hPa are shown for when the DOFS  
26 are larger than one for this altitude region. There is a slight bias of -2.7 +/- 1.5 per mil between  
27 TES and AIRS as shown in the top panel. The calculated and actual (RMS difference between  
28 AIRS and TES) uncertainties are shown and are approximately 30 per mil, primarily driven by  
29 the uncertainty in the AIRS based estimates as the TES based estimates have an uncertainty of  
30 approximately 15 per mil. Figure 5 shows a direct comparison of the AIRS and TES data. The  
31 correlation is about 0.89 and the one-to-one line (solid line) overlaps this distribution. However



1 the lowest values likely diverge from the one-to-one line, possibly because the vertical  
2 distribution in the sensitivity depends on the amount of HDO and hence we should expect  
3 differences between the TES and AIRS deuterium measurements for these lower-sensitivity  
4 retrievals.

5 A comparison of the AIRS and TES HDO/H<sub>2</sub>O ratio for five single global surveys taken  
6 between 2006 and 2010 (one global survey per year during boreal summer) is shown in Table 1  
7 and indicates that the overall bias varies between -2.7 to 3.7 per mil. Using all 5 TES global  
8 surveys that are summarized in Table 1 we can construct how AIRS and TES compare as a  
9 function of latitude as shown in Figure 6. Figure 6 is constructed by averaging the difference  
10 between TES and AIRS observations within 5 degree latitudinal bins. The mean bias across  
11 latitudes is ~-2.6 per mil. The error bars shown on the difference is the error on the mean, which  
12 is the Root-Mean-Square (RMS) of the differences divided by the square root of the number of  
13 co-located observations; as this error bar is a measure of precision for each latitude bin, this  
14 comparison demonstrates that there are variations in the comparison that are larger than the  
15 precision and are therefore related to systematic errors in either the TES data or AIRS data or  
16 both. Variations in these systematic errors can be seen in the latitudinal variability, which has an  
17 RMS variation of ~7.8 per mil for the different latitude bins but can vary by as much as ~15 to  
18 ~+15 per mil in the tropics. Typically these variations are due to a combination of uncertainties  
19 in the spectroscopy along with temperature, water vapor, and surface properties; they may also  
20 be due to "smoothing error" which is related to how differences in the vertical resolution affect  
21 the tropospheric average of the deuterium content shown in these figures (e.g. Worden *et al.*  
22 2004). This 7.8 per mil variation across latitudes is about the same as the reported accuracy of  
23 the Aura TES delta-d observations that are based on comparisons of TES data with surface and  
24 aircraft measurements (Worden *et al.* 2011; Herman *et al.* 2014). We therefore report the current  
25 accuracy of the AIRS data to be ~7.8 per mil. We expect future comparisons between these data  
26 and those from aircraft or revisions to the AIRS retrieval approach will modify this estimate of  
27 the accuracy.

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30 **8) Conclusion**  
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**Deleted:** The calculated errors are calculated during 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<sub>2</sub>O 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.

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**Deleted:** These comparisons therefore show that the AIRS estimates of the HDO/H<sub>2</sub>O ratio are robust as the calculated and actual uncertainties are consistent with an accuracy comparable to observations from TES.

1 This paper describes the vertical resolution and error characteristics of retrievals of the  
2 deuterium content (or the HDO/H<sub>2</sub>O ratio) of water vapor using AIRS radiances and then  
3 evaluates the consistency between AIRS and TES retrievals of HDO and H<sub>2</sub>O. We find that the  
4 AIRS and TES deuterium content for the lower-troposphere (750 – 350 hPa) are consistent, or  
5 within their calculated uncertainties, for the 5 year period in which TES observations span the  
6 globe (2006-2010). We find the total uncertainty for a single AIRS observation is ~30 per mil  
7 with an accuracy of ~7.8 per mil. These uncertainties can be compared to the observed total  
8 variability, which can range from approximately -350 to -50 per mil over the whole globe, as  
9 observed by the Aura TES data (Worden et al. 2006) and shown in Figure 3 for AIRS data.

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

## 20 Acknowledgements

22 The research was carried out at the Jet Propulsion Laboratory, California Institute of  
23 Technology, under a contract with the National Aeronautics and Space Administration.

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Table 1: Comparison between averaged TES and AIRS HDO/H<sub>2</sub>O 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 ... [1]

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Date

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1 Table 1: Comparison between averaged TES and AIRS HDO/H<sub>2</sub>O ratio (750-350 hPa). The units  
 2 are in parts per thousand relative to Standard Mean Ocean Water. The second column shows the  
 3 expected RMS based on the uncertainties of the TES and AIRS data. The third column shows the  
 4 actual RMS difference between TES and AIRS. The last column shows the mean difference.

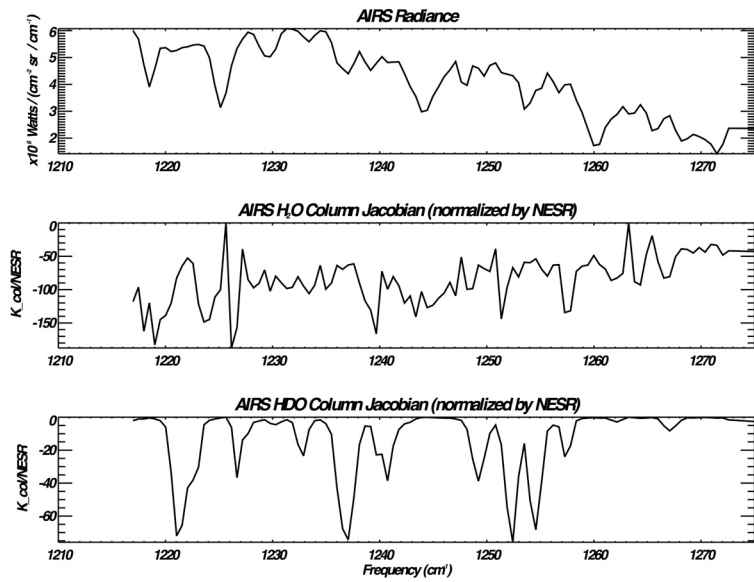
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<u>Date</u>	<u>Expected RMS</u> <u>(per mil / SMOW)</u>	<u>Actual RMS</u> <u>(per mil / SMOW)</u>	<u>Mean (TES-AIRS)</u> <u>(per mil / SMOW)</u>
<u>2006-06-01</u>	<u>31.1</u>	<u>30.6</u>	<u>-2.7 +/- 1.5</u>
<u>2007-06-02</u>	<u>30.0</u>	<u>31.9</u>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

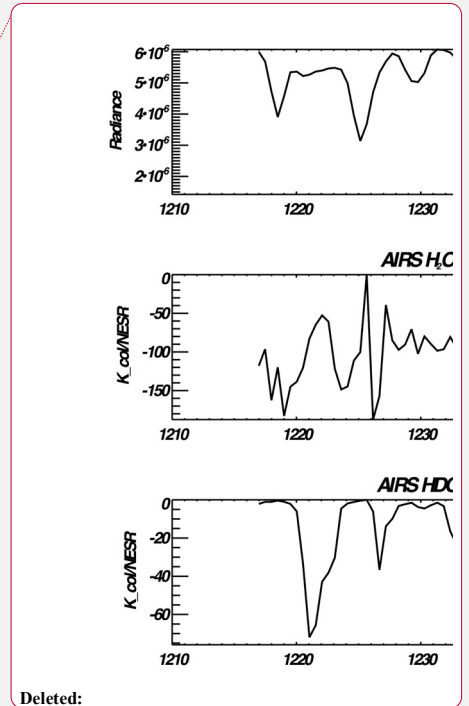
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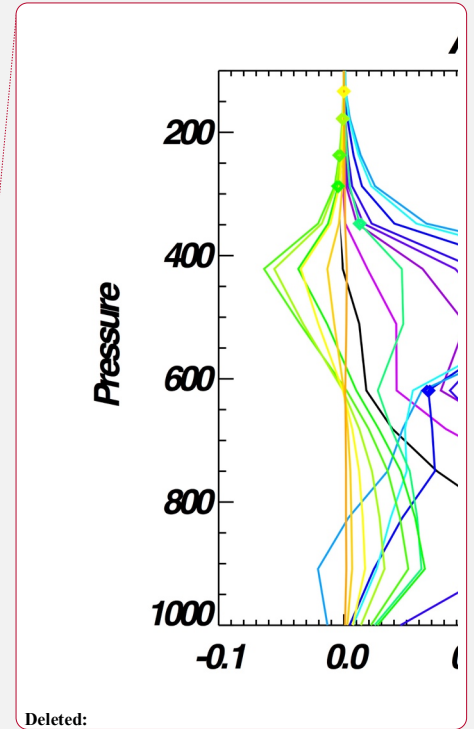
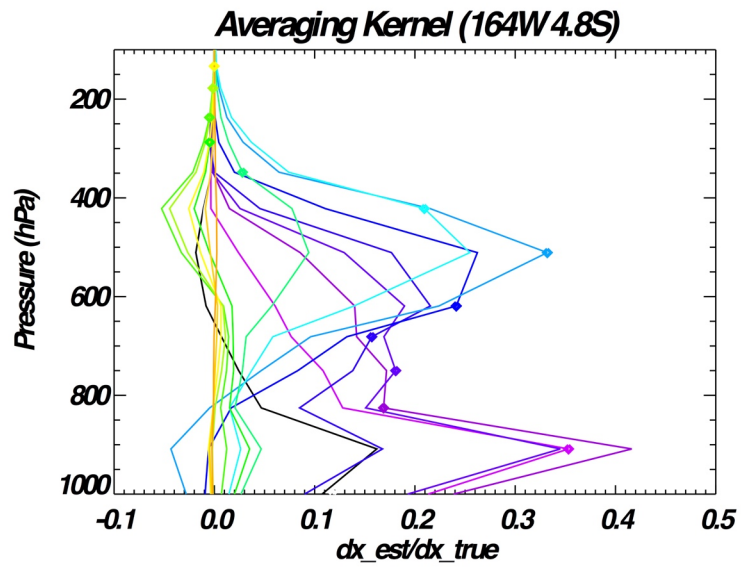
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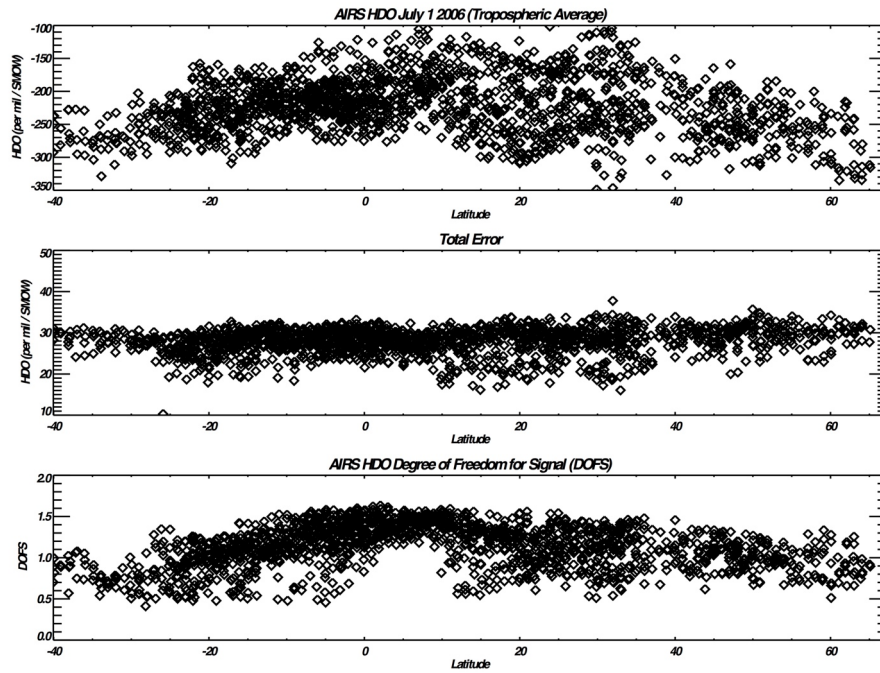
Figure 1: (top) AIRS radiance at approximately 8 microns for a typical tropical scene. (middle) The total column (log) Jacobian for H<sub>2</sub>O normalized by the AIRS NESR. (bottom) The total column (log) Jacobian for HDO normalized by the AIRS NESR.





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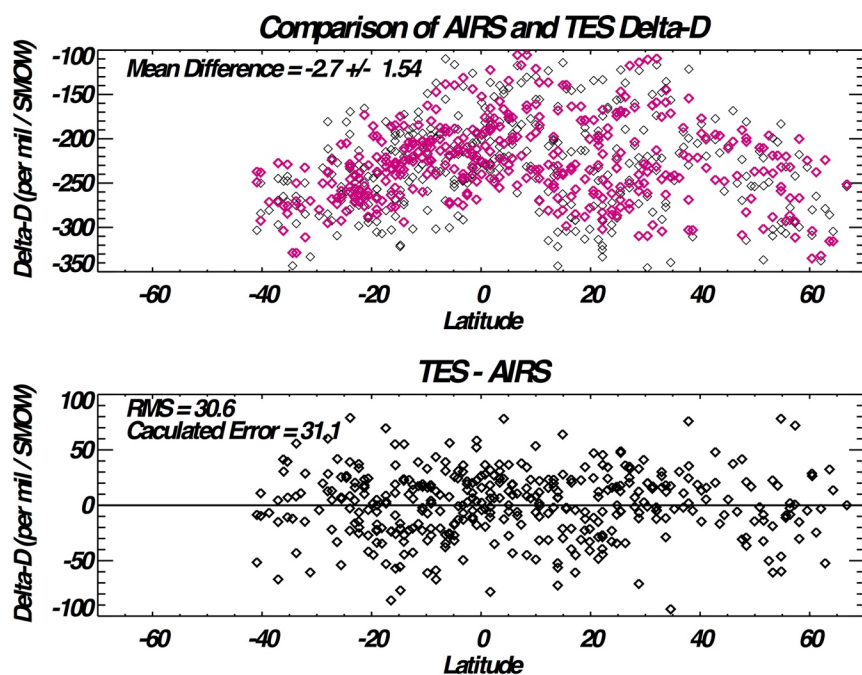
Figure 2: The rows of the averaging kernel matrix for the HDO retrieval corresponding to the radiance shown in Figure 1. The different colors and symbols are used to indicate the pressure levels corresponding to each row of the averaging kernel matrix.



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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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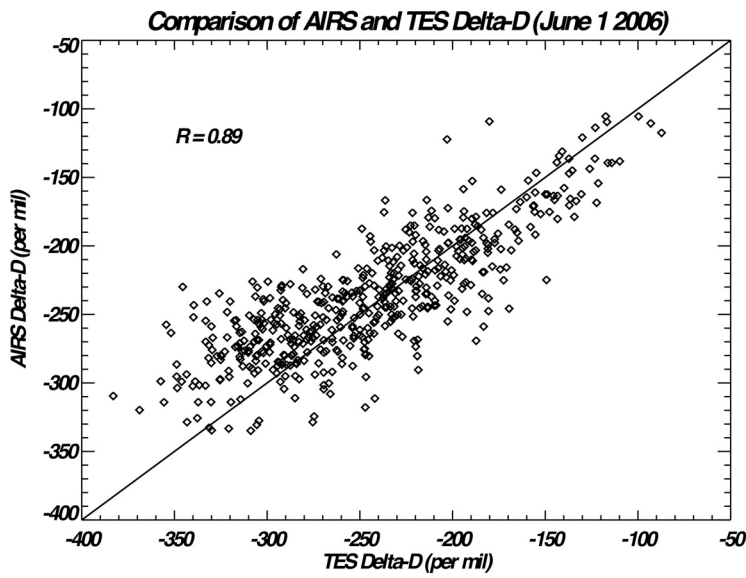


2 Figure 4: (top) Comparison of AIRS (red) and TES (black) delta-D for June 1 2006 (~600 co-  
3 located observations). (bottom) The differences (after bias subtraction) between TES and AIRS  
4 delta-D measurements.  
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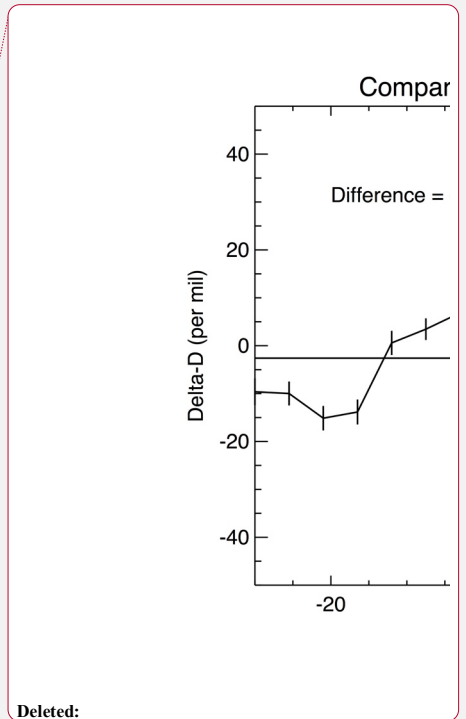
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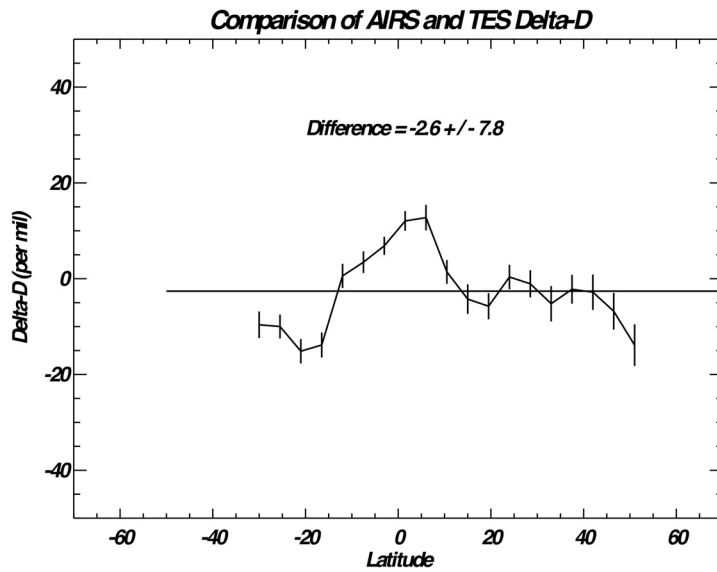
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2 Figure 5: Comparison of the AIRS and TES deuterium content. The solid line is the one-to-one  
3 line.

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

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1 I would like to greatly thank both reviewers for their detailed review and comments. Reviewing and  
2 editing these papers is quite a bit of (effectively voluntary) work and both reviews really went into  
3 great detail on fixing the presentation. With respect to the comment on “minimalism”, I actually was  
4 striving for minimalism in this paper but apparently overshot my goal! ☺. For example, I did not  
5 want to write (yet) another paper full of the optimal estimation description in all of its gory, (or  
6 glory?) equation detail but instead report on the basic notions..... that the AIRS radiances can be  
7 used to generation global deuterium content retrievals and that their vertical resolution is about  
8 the same as TES but with slightly poorer uncertainties, and that we will soon produce a long record  
9 of the data that spans most of the globe and can hopefully produce scientific awesomeness.

10 Again, thanks for the review. Below are the comments and my responses.

### 12 Response to Reviewer 1

13 General Comment: This study presents the application of an existing retrieval methodology of  
14 HDO/H<sub>2</sub>O vertical profiles originally applied on TES, on AIRS thermal infrared measurements. The  
15 authors briefly remind the retrieval methodology, describe the error and sensitivity, and show a  
16 comparison with co-located TES retrievals. In my view, this is a welcome study as the capabilities of  
17 AIRS sensors for HDO/H<sub>2</sub>O ratio retrievals were unknown/not tested, and the sampling  
18 characteristics of AIRS offer great potential for isotopes related studies. The manuscript is short  
19 and generally convincing but the presentation is too minimalist and should be improved. Some  
20 discussions on previous improvements in characterizing HDO/H<sub>2</sub>O pairs retrieval is missing. I  
21 list a few comments which should be easily resolved by the authors.

### 22 Specific Comments:

- 23 • Introduction: A short introduction on water isotopes, their usefulness and a description on  
24 what are the remote sensing capabilities to observe HDO/H<sub>2</sub>O ratios in the free  
25 troposphere would be useful to strengthen the importance of this work and to smooth the  
26 feeling of reading a purely technical report.

27 Response: I added a paragraph at the front that describes a bit of history on water isotope  
28 measurements, and how these vapor based measurements have helped address global  
29 water / carbon questions.

- 30 • P2, Line 19: estimates of HDO/H<sub>2</sub>O ratios and not HDO

31 Response: Added “and their ratio”. We actually do retrieve HDO and H<sub>2</sub>O separately even  
32 if the retrieval setup optimizes the ratio.

- 33 • P2, Line 20: Why only summertime TES global survey’s? Do you mean boreal summertime?

34 Response: added boreal and added a statement about current limited processing  
35 capabilities



- 1 • P2, Line 23: “We then compare the AIRS and TES data to evaluate and quantify the  
2 calculated uncertainties of the AIRS data” - To evaluate and quantify the calculated  
3 uncertainties sound a little odd. This needs to be rephrased.
- 4 **Response:** removed “and quantify”
- 5 • This paper is relatively short and yet there is a lot of statements about futures publications  
6 (P2, L17-18;P2, L23-24;P5, L29 – P6,L8). Some of them could be removed.
- 7 **Response:** Removed most of these references where appropriate and modified some of the  
8 language about the utility of the 12 micron band for constraining atmospheric temperature.
- 9 • P3, L8: There is a redundancy here of the statement that TES is part of the A-Train, it was  
10 just said in the previous sentence.
- 11 **Response removed**
- 12 • P5, L9: “This retrieval algorithm can use radiances (..) to quantify and characterize  
13 geophysical observables appropriate for the corresponding radiance.” – What is an  
14 appropriate geophysical observable? To retrieve different geophysical parameters?
- 15 **Response:** changed “appropriate” to “that affect”. I think this wording is appropriate but  
16 terse. I can also add another line such as (e.g. the ozone concentrations affect radiances in  
17 the 9.6 micron ozone band) but that seems too wordy.
- 18 • P5, L16-17: “in order to ensure that [the retrieval of] the ratio is optimized, as opposed (..)”  
19 [missing]
- 20 **Response fixed**
- 21 • P5, L29 – P6,L8: All this part describes the importance of including the 12 microns  
22 radiances for the methane retrieval. That is not interesting in the frame of this paper.
- 23 **Response (fixed in above response, hopefully ☺).**
- 24 • P6, L17-19: Jacobians have not be defined. What does the -50 treshold represent? How is it  
25 calculated?
- 26 **Response:** I added the definition for a Jacobian and changed the language around.. basically  
27 2% is equivalent to 1/50... 1% = 1/100 etc.
- 28 • P6, L22: “[...] partial derivative of the estimate relative to [partial derivative] of the true  
29 state”. Or maybe in a language more accessible to potential users not familiar with optimal  
30 estimation: “the response of the retrieved state to perturbations of the true state”
- 31 **Response:** changed

- 1 • P6, L23: It is confusing to translate the example in terms of HDO/H<sub>2</sub>O ratios since the  
2 averaging kernels are for HDO.

3 **Response** thanks for pointing this one out.. I adjusted the language accordingly and added a  
4 sentence about how the information about HDO/H<sub>2</sub>O is limited by HDO; I also added a  
5 reference.

- 6 • P6, L28-29: Schneider et al., 2012 proposed an a posteriori methodology to characterize the  
7 joint retrieval of H<sub>2</sub>O and HDO. The method allows to transform the products obtained in  
8 the log(H<sub>2</sub>O),log(HDO) space into a proxy state log(H<sub>2</sub>O),δD which is very useful for  
9 characterization. Moreover, the HDO/H<sub>2</sub>O ratio product is often used in pair with H<sub>2</sub>O it is  
10 therefore important to discuss the differences of sensitivity of H<sub>2</sub>O and HDO/H<sub>2</sub>O ratios.  
11 This is missing here.

12 **Response** I added language on how the averaging kernels for H<sub>2</sub>O are different than that for  
13 HDO and that Schneider et al discusses an approach to use these data with simple models  
14 while accounting for the different sensitivities.

- 15 • P7, L13-L15: There are a lot of measurements within the tropics with DOFS between 0.5 and  
16 1 so I wouldn't generalize this situation to the whole tropics. This might be valid only for the  
17 averaging kernels shown.

18 **Response:** adjusted the language .. now we say “many” which implies “not all”

- 19 • P8, L6->L11: All this part would better fit in the error characterization part

20 **Response:** moved

- 21 • Comparisons of AIRS and TES retrievals - In order to be really convincing, this part needs to  
22 be completed.

23 - Would it be possible to show a scatter plot of AIRS versus TES?

- 24 • - What is the correlation between AIRS and TES retrievals?

25 **Response:** I am not that convinced this is a meaningful figure as it is the difference  
26 between AIRS and TES that can be used to determine if the AIRS data is (relatively) well  
27 characterized. Having said that I have included it here in case readers find it useful. The  
28 correlation for this day is 0.89.

- 29 • - Because this kind of product is used in pairs with humidity retrievals it is also interesting  
30 to show that both sounders show the same humidity-δD information and not only δD.

31 **Response:** I dont think this comparison is of use to this specific paper as it shows that the  
32 pairs generated by AIRS are similar to those from TES but slightly different, as expected  
33 because the sensitivity and errors are different. For this reason I would prefer not to show  
34 here, but will show in subsequent papers when we start looking at the science!

- 1 • - I didn't understand the error assessment reasoning. The mean bias across latitude is -2.6  
2 permil, later on the authors assess the RMS to be 7.8 permil then the authors say the  
3 accuracy is 7.8 permil. Is this a mistake or do I miss something? The language between  
4 accuracy and precision should be clarified.  
5 • - What about the latitudinal variations of the bias which are greater (-15 to 15 permil) than  
6 the mean standard error? It looks like there is a latitudinal bias, could it be caused by some  
7 dependence on temperature or humidity content?

8 **Response:** I attempted to clean up the language here, hopefully it's a bit more clear! I also  
9 added language that the latitudinal variations are typically due to uncertainties in  
10 temperature, water vapor, and spectroscopy, as well as differences in the vertical  
11 resolution.

- 12 • - Could you plot the data in Figure 5 until 40°S as in the previous figure?

13 **Response:** Done!

- 14 • The conclusions could be more developed. One of the interest of this paper lies in the  
15 development of a HDO retrieval methodology from AIRS data which was unknown and  
16 opens great perspectives for users interested in such measurements. In this context, a word  
17 on the future plans of the authors on processing more AIRS data, or not, would be  
18 interesting.

19 **Response:** Added a paragraph on current and future plans with respect to building an ESDR.

- 20 • P9, L8: Please reference the natural variability of  $\delta D$

21 **Response:** Added statement about Figure 3 and cited a TES paper.

#### 22 **Technical corrections**

- 23 • Abstract, L17: Northern instead of N; • P1, L28: a verb is missing (fixed)  
24 • L29, degrees (fixed)  
25 • P4, L30 : Description of Retrieval Approach -> Description of the retrieval approach (fixed)  
26 • P5, L29 : (e.g. Figures 1-4). (fixed)  
27 • P7, L4: add degrees to latitude (fixed)  
28 • P7, L8: use the delta Greek notation  $\delta$  (this is stylistic, I have added "or  $\delta$ " instead)  
29 • Figure 4: A legend is missing, what is TES and what is AIRS? (fixed)

30

1 Reviewer 2

2

3 **General Comment**

4 As this study is targeting the preparation of a new Earth Science Data Record covering AIRS  
5 HDO/H<sub>2</sub>O observations, it clearly has a high scientific significance. The manuscript itself is clear  
6 and concise, but I would agree with Reviewer #1 that the presentation is indeed somewhat  
7 "minimalistic" and could be extended and improved. Please carefully follow suggestions and  
8 comments provided by Reviewer #1 and those listed below so that the paper can be published  
9 soon.

10 **Specific comments**

11 

- p3, l4: The AIRS swath width is 1650 km (Aumann et al., 2003) rather than 1250 km.

12 Response: (fixed)

13 

- p5, l25-26: Although the AIRS noise is characterized well for individual channels, in  
14 other work I noticed noise can be spectrally correlated between neighboring channels,  
15 which is due to the 1-D linear detector arrays of AIRS sharing the same electric module  
16 (Pagano et al., 2008). This may be too specific to discuss in your paper; I just wondered  
17 if you considered this?

18 Response: We have not explicitly addressed this issue and in fact the same is true with the TES  
19 data because the data are apodized but the calculated errors assume the noise is random (or not  
20 apodized). On the other hand the apodization is accounted for in the TES retrievals when we  
21 calculate the forward model radiance. In contrast with the TES data where we can account for  
22 the apodization it is not clear how to account for these noise correlations in the AIRS data.  
23 Instead we added a statement that the noise is assumed to be random as we are unable to account  
24 for correlations between channels. The effect of this assumption is that the calculated errors will  
25 be too large and is therefore a conservative estimate of the uncertainties.

26 Pagano, T. S., Aumann, H. H., Schindler, R., Elliott, D., Broberg, S., Overoye, K., and Weiler, M. H.:  
27 Absolute radiometric calibration accuracy of the Atmospheric Infrared Sounder (AIRS), in: Proc.  
28 SPIE, vol. 7081, doi:10.1117/12.795445, 2008.

29 

- p7, l20-29: Are the HDO retrieval results correlated with the simultaneous H<sub>2</sub>O re-  
30 trievals? Does the AVK matrix show any correlations between these retrieval variables?

31 Response: Yes! These correlations are addressed 1) in model comparisons by applying the  
32 averaging kernels for both HDO and H<sub>2</sub>O to the model (e.g. Risi et al. 2013) or 2) by calculating  
33 the resulting error (e.g. Worden et al. 2006) and including that in the error budget, or mitigating  
34 further by 3) projecting to HDO-H<sub>2</sub>O pairs as discussed by the first reviewer. I have discussed the  
35 pairing approach based on the first reviewers comments and will add the Risi reference as well.

1 Fig. 2: Maybe show also the integral of the AVKs, to indicate the amount of measurement  
2 information in the retrieval results? (Fix "are used to indicate" in the caption.)

3 Response: Fixed caption. The integral of the AVKs (or trace actually) is shown in the bottom  
4 panel of Figure 3 and discussed in the text.

5 Fig. 4: A legend/definition of the colors used for the plot on the top seems to be missing.

6 Response: Fixed!

7 Technical corrections  
8 p1, 117: N. -> Northern (also in other places) (fixed)  
9 p1, 122: ...reduced spectral resolution of AIRS (for clarity?) (removed sentence as it was confusing  
10 to have in the abstract)

11 p1, 124: Suggest to remove reference (Worden et al., 2004) from abstract. p1, 127-28: Please fix  
12 incomplete sentence. (see above)

13  
14 p1, 129: Add degree symbols to "30 S and 50 N" (also in other places)? I have added the word  
15 "degrees" instead.

16 p2, 12: The copyright statement "All rights reserved." is not allowed in the given form, I think, please  
17 see [https://www.atmospheric-measurement-techniques.net/about/licence\\_and\\_copyright.html](https://www.atmospheric-measurement-techniques.net/about/licence_and_copyright.html) for  
18 details.

19 Response: I have to use this copyright for JPL during the submission phase. Once / if the paper is  
20 accepted I put in another form where JPL puts in a modification to the Copernicus agreement.

21 p2, 14: "Introduction:" -> "Introduction" p3, 111: PAN, -> PAN  
22 fixed

23 p3, 122: Earth Science Data Records (ESDR's) -> ESDR's (acronym was already introduced)  
24 fixed

25 p4, 125: "a version of the v4 AIRS" -> "version 4 of the AIRS" (?) (fixed)

26 p5, 16: will only briefly summarize (?) (fixed)

27 p5, 19-10: Not sure if "...appropriate for the corresponding radiance." is a good phrase here?  
28 (changed, see comment from reviewer 1)

29 p6, 14-6: Remove redundant sentence. (fixed)

1

2 p6,131: Change date format to "1 July 2016" (also in other places); I think this is a US Versus Europe  
3 date thing ☺. Can I keep as is? Its like asking me to drive in the left lane ☺.

4 p7,12: we can only (?) (fixed)

5

6 p8,114: indicate s (fixed)

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