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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Estimate of bias in Aura TES HDO/H_2O profiles from comparison of TES and in situ HDO/H_2O measurements at the Mauna Loa Observatory" *by* J. Worden et al.

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General Comments to Both Reviewers: Both reviewer 1 and reviewer 2 state that the assumptions used in this analysis need to be better articulated and characterized; this has been a difficulty in writing this paper given the boutique approach in using PBL variability to construct vertical profiles and characterizing the impact of this approach on the error analysis. We hope this next draft better states these assumptions and the consequences on the results!. For example, we have revised our error analysis to better quantify the errors in the differences between the in situ measurements and the TES data; this error analysis uses the approach described in Worden et al. [2006] and

H. Worden et al. [2007]. We believe we have also better characterized the impact of the primary assumptions used in our comparisons on the bias estimate. Because the bias estimates derived from our 3 comparisons are much closer together than expected from our calculated uncertainties it is quite possible that our errors are too conservative and should in fact be smaller; however revision of the bias estimate will require more data. Finally, we better quantify they bias estimate and its errors by computing a lower tropospheric average between the TES estimate and the constructed true profile from the in situ data. The bias is adjusted until this difference is less than 0.3 per mil. The uncertainties are calculated using the revised error analysis and the bias estimate has been changed from 5.6% to 6.3% in this version of the manuscript.

There are two primary assumptions in this analysis (1) the isotopic composition of the day time free tropospheric air parcels is similar to the isotopic composition during the night and (2) we can use the TES H2O and pressure grid to map the picarro H2O and delta-D values to a grid that can be used for comparing the in situ data to the remotely sensed data. Both of these assumptions are required in order to make use of the diurnal variability of the boundary layer to construct a 'profile' of H2O and HDO that can be compared to a remotely sensed estimate.

There are two ways in which assumption 1 could provide an incorrect assessment of the bias estimate: (a) if the actual daytime free-tropospheric delta-d values were biased high relative to night-time air with similar H2O concentrations due to mixing processes and (b) the variability of the night-time air for a range of H2O values is larger than expected.

In order to build a better argument for assumption (a) we have swapped section 4 with Section 3. Section 4 shows that the TES data have to be corrected by at least 0.056 in order for the TES lower tropospheric delta-d over the subtropical pacific to agree with the distribution measured by the in situ data. We believe this is a robust assumption because both data sets measure a combination of free troposphere air and air in the upper boundary layer. What we cannot say with this comparison is whether the bias should be larger than 0.05 as values up to 0.09 would also be acceptable if the only criteria is that the distributions have to completely overlap. We also find that if we artificially increase the night-time values used to estimate daytime free-tropospheric delta-d by, for example, 50 per mil that the our bias estimate decreases from about 0.06 to less than 0.02 which is inconsistent with this result. Secondly, we believe we are addressing (b) by including night-time measurements that are before and after the daytime measurements and including the variability in these measurements as the uncertainty of the corresponding delta-d / H2O pair used for comparison with the TES data. This discussion is now in the text (Section 5.3). Note that much lower values of the night-time delta-d / H2O pairs would not be expected from the distribution of values measured by Picarro and LGR. However we cannot rule this scenario out but merely state that it is unlikely.

The other primary assumption is the use of TES H2O and pressure to map the picarro H2O and delta-d values to a pressure grid that can then be used for comparing the in situ data to the remotely sensed data. This assumption results in an interpolation error that we estimate to be small enough to ignore ($\sim$6 per mil as discussed in Section 5.3). However, this assumption does show that we need to assume that the TES H2O errors have to be included in the error budget (Equation 4 Sections 5.0 and 5.3) since we are substituting the “true H2O” with the TES H2O. The revised error analysis included in the paper now characterizes this assumption and we find that the TES H2O errors do not affect our conclusions too much because, as discussed in Worden et al., 2006, the retrieval errors of the H2O and HDO concentrations are mitigated when constructing the ratio.

Response to Reviewer 2

We would like to thank the reviewer for your comments especially given the depth of your knowledge related to the meteorological conditions around Mauna Loa. Many of these comments are related to understanding the different meteorological effects that could affect our comparisons between the TES HDO/H2O estimates and the in situ

data. We have added a summary of this potential affects as well as the Barnes et al. reference to the paper in order to address these issues.

Comment: How representative are the data at the Mauna Loa Obser vator y (MLO) to the sub- tropical free troposphere? The TES observations shown in the paper were taken during daytime and have a strong gradient in deltaD and likely also in water vapor above Mauna Loa. While moist layers at various heights are not uncommon in the trop- ics, there is also a warm surface in the center of the range of heights to which the lower/mid-tropospheric TES HDO/H2O measurement is most sensitive. Would any of these effects – in par ticular the presence of the surface in the middle of the region of sensitivity – make the bias estimate from MLO less than representative of general subtropical or global measurements?

Response: If the assumption that the bias is due to spectroscopy is valid (e.g. Webster private communication and Toth private communication) then we would expect that the bias estimate calculated for conditions at Mauna Loa should be valid globally (within the expected uncertainty). However, while we might expect this result theoretically, we still need to show it empirically but will not be able too until there are more data to test this assumption against. Note that a spectroscopic bias is indistinguishable from a bias in estimated layer column amount. Consequently, this bias does need to be corrected by the sensitivity of the estimate as discussed in the paper.

Comment: The "Constructed True" water vapor profile is taken from the TES H2O profile. TES seems to have limited vertical resolution, so that I would interpret this profile as being a smoothed version of the "true" profile. I would have expected a nearly-well mixed layer near the surface at mid-day close to the in-situ value, with drier free tropospheric air above whose mixing ratio would be close to that of the Hilo sounding at the level of MLO. (See e.g. the MLO radiosonde sounding in ïňĄgure 1 in Barnes et al (2008) at http://www.agu.org/pubs/crossref/2008/2007JD008842.shtml which has a relatively well-mixed layer near the surface. My impression is that TES smooths the sounding even more than the Lidar does in that ïňĄgure at lower layers.)

Would your HDO/H2O retrieval be much different if your "Constructed True" sounding had a different shape, with a contrast between a well-mixed layer near the surface and a drier free troposphere?

Also, in my view, the study would have benefitted greatly from having launched radiosondes from MLO itself synchronized with the five TES overïňĆights. Perhaps, this wasn't done for manpower, cost or other reasons. However, it would have removed a significant source of uncertainty in my view. It may be that the broad vertical averaging inherent in the TES HDO/H2O estimate renders it insensitive to the issue raised here, but I believe that this should be mentioned in the paper.

Response: It is interesting that the lidar shows an enhanced layer of water above Mauna Loa that appears to be consistent with the enhanced water observed by TES relative to the nearby sonde. The calculation of the averaging kernels depends on the estimate being close to the truth. If the true water is significantly different from the estimate then the averaging kernel calculation is not valid. However as shown in the TES H2O and in situ comparisons, the TES and in situ estimates agree generally within the TES error AND with the measurements in the Barnes et al paper (now referenced in Section 5.1). Consequently, this paper re-affirms that our H2O measurements appear to be valid (i.e., within expected errors). I agree that co-launched sondes would have been desirable; however we did not have the foresight to include these sondes in our budget.

Comment: Are the night-time MLO H2O/HDO values characteristic of free tropospheric air above MLO at mid-day? Perhaps, checking Hilo soundings 12 hours before and after the TES overïňĆights could shed light on this for H2O if not HDO. Also, MLO is about 800m belowthe top of Mauna Loa, so that even nighttime air is likely blowing down the mountain rather than subsiding directly from the free troposphere. Is this important?

Response: This comment is addressed in the general response.

Comment: Are the daytime MLO H2O/HDO values characteristic of those in the moist layer above MLO? This seems quite plausible.

Response: Most likely yes.. however what is more important for constructing the “true” HDO/H2O profile is that the variability of the HDO/H2O with respect to H2O is captured by the in situ data not the absolute amount.

Comment: Are the intermediate mixtures of dry and moist air (and their HDO/H2O) ratios observed at MLO characteristic of the mixtures above MLO during the TES over pass? Of these three, this seems the least likely to be true. The mixtures seen by the TES ïňĆight are between free tropospheric air blowing in and the plume of boundary layer air rising over the mountain, not between different proportions of boundary layer air ad-vecting up the mountain during the morning and early afternoon (themselves probably representing mixtures of boundary layer air and entrained free tropospheric air from lower down the mountain). If you had a radiosonde sounding with a well-mixed surface layer capped by a strong inversion, this issue would be much less important because the mixtures would occupy only a small range of pressures. However, with the smooth TES H2O proïňĄle, these mixtures seem to be dictating at least the lowest two levels of the sounding.

Response: This mixing might be best observed for the October 20th comparison which shows significant variability in the isotopic composition during the daytime. It is not likely that the air observed by TES is represented by this rapid change at Mauna Loa (as you point out). However, what is important for the comparison is whether the isotopic composition varies with H2O in a consistent manner. As noted earlier, if mixing were significant for the more dry air parcels that are observed by TES AND are within the altitude range for which the TES HDO estimates are sensitivity, then we would expect that the constructed “true” profiles would be more enriched then expected. As noted earlier this would imply a smaller bias correction which would be inconsistent with the comparison of distributions shown in what is now Figure 2.

Comment: I think it would be interesting to see if your HDO and H2O in situ data form a mixing line. This would at least tell us something about the mixtures you observe at MLO. Could you make additional scatter plots of HDO (vmr) vs. H2O (vmr) for the data in ïňĄgures 5, A2 and A6 to show whether these mixtures lie on a mixing line between your night-time (nominally free tropospheric) values and your mid-day values?

Response: This is the subject of a subsequent paper (Noone et al. submitted). The representativeness of the delta-d / H2O pairs appears to be the main concern addressed here and we respond to this in previous comments.

Comment: The strength of the wind atop Mauna Loa could change the composition of the air atop the mountain (and that observed during the TES overïňĆight) considerably. On a still and sunny day, a plume of boundary layer air advected up the mountain could accumulate above the top of the mountain. On a windy day, such a plume would blow off much more readily if it ever reached the top of the mountain. As a result, free tropospheric air would likely have more inïňĆuence on the composition of the air above MLO. Based on the H2O VMR observed on 5 Nov, I would infer that that day was windier than the other two. It seems worth mentioning the wind conditions on each day.

Response: I think the point of this comment is that there are many meteorological effects that could affect the H2O and thus HDO/H2O distribution. However, its not clear to me how our conclusions would change if wind measurements were shown as again this would impart variability in the HDO/H2O in situ distributions which in turn would affect our error estimates for the "true" distribution. As discussed previously though, we include this in the discussion in the paper. In addition, note that the expected error for the lowest pressure Nov 05 delta-d/H2O pair is larger than the rest.. consistent with your inference.

Minor Comments:

Minor comments/suggestions (all page numbers star t w/253):

p. 56, l21: Specify whether the 1 percent uncertainty of the bias correction is absolute or relative. Similarly for p. 60, l6 (abs. or rel. precision) and l8 (abs. or rel. bias).

Response: Added precision and accuracy into abstract (note the change). I did not find error estimates on p 60 but changed these values where appropriate

p. 57, bottom: Boxe et al 2010 not in references.

Response: Fixed

p. 58, l20: "... to _proïňĄles_ of HDO and H2O."

Response: Fixed

p. 58, l23: "... kernel and _an_ a priori constraint ..."

Response: Fixed

p. 60, l20: Give a number (3.2?) instead of saying "the next section". Response: Fixed

p. 62, l21: "error on this estimate" – I assume this is an upper bound on the error. If so, it would be useful to say "error bound" or "uncertainty". It would also be useful to make clear that this whether this is a relative or absolute uncertainty.

Response: Changed to total uncertainty and indicated that the uncertainty is taken from the TES product files.

p. 62: Could you show the TES-inferred variability in H2O and possibly HDO/H2O for the curtain of observations passing over MLO to make this clear to the reader? You should also include a depiction of Aura's path over MLO in ïňĄgure 2.

Response: I think showing the cloud distribution from MODIS as well as the nearby sonde measurements make this point pretty clear. I added a cross to the approximate location of the Mauna Loa observatory (by eyeballing a google map) onto the MODIS image. With my current toolset I cannot easily add an orbit path onto the MODIS imagery due to the way the image is warped for presentation.

p. 63, eqn 2: Do you need equation 2? Can't you just say "We map the in situ H2O and HDO data onto a vertical pressure grid using the H2O values and pressure levels observed by TES during its overïňĆight. The set of in situ values which lie within 5% of the H2O value observed by TES at a particular TES pressure level are averaged to give the constructed true values of H2O and HDO at that level." or something like that. I found the P_{TES}(H2O_{in situ}) notation a bit confusing.

Response: I agree with this assessment, equation removed and wording copied verbatim into section.

p. 63, l14: Should be ïňĄgure 5, not 4.

Fixed

p. 63, l18: I think you mean to say "lower than 0.001 VMR are not _seen_ by ..." Saying "are not measured" could be confused for asserting that the instuments are not capable of measuring such concentrations.

Language adjusted to indicate that the instruments did not observe these quantities during this time period.

p. 63, l20: Is 5% big enough? Should you use a ïňĄlter (other than top hat) in H2O VMR space to compute the averages? Would it be more robust to average observations onto a H2O mixing ratio grid and then construct your true sounding by sampling/averaging from there? Are you oversampling from relatively steady periods in your in situ measurements?

Robust in this context means that there are enough data points to represent variability of the HDO/H2O measurements for the range of H2O measurements. I went back and checked and found that a 5% threshold provided between 30-90 H2O / delta-D pairs for 2 of the observations. However, I had to increase the threshold to 10% for the October 19 date in order to obtain at least 10 pairs for each HDO value. A more sophisticated filter could be used but I don't see the point as long as the errors from the pairing are

small enough to make a comparison reasonable and I have reasonably captured how the variability affects the errors. I have changed the text accordingly to reflect this new threshold and to better explain the choice

p. 63-64: Could you give some indication of what fraction of the integrated sensitivity to HDO/H2O comes from the region spanned by the ïňĄve points shown in ïňĄgure 3?

These numbers are shown in the averaging kernel plots.

p. 64, l17-18: Fig. 3, not ïňĄgure 2.

Fixed

p. 66, l21: Insert q_HDO as in "where q_HDO is the volume mixing ratio ..." This variable appears in my Word document but somehow got deleted in the online PDF. I will check the next uploaded version to ensure this is inserted properly.

p. 71, l25: "preparation" not "preperation"

Fixed

p. 74, ïňĄg 1: Is the data around day 305 missing? If so, don't plot it.

The data are missing and in fact there are several data gaps of varying length throughout the shown time series. I would agree with you about not plotting the data gaps if I were interpreting the long-term time variability. However, since I am not interpreting the long term time variability I think it is reasonable to interpolate through the data gaps in the figure.

p. 75, ïňĄg 2: Add locations of MLO, top of Mauna Loa, Hilo and Lihue along with box for footprint of TES observation above MLO and line for path of Aura over pass. Same for A1 and A5.

Note that I am making these additions to the MODIS JPEG images using powerpoint and then googlemaps to eyeball the locations of each site. The reason for this approach is that I do not have coordinates for each pixel of the MODIS JPEG images; there might be a way to obtain this information but I do not know how and in any case the added information for the amount of work required would be minimal. For this reason I cannot put in the Aura orbit but I can put in the MLO, Hilo, and Lihue locations.

p. 76, ïňĄg 3: The HDO/H2O prior seems pretty far off. Does this affect the quality of the HDO/H2O estimate from TES?

Only if the retrieval did not converge. These retrievals converged as indicated by the radiance residual RMS and Mean relative to the noise and have sufficient sensitivity to observe the vertical distribution of the HDO/H2O ratio as indicated in the data section. I have added the convergence statement in the data section.

p. 76, ïňĄg 3: Could you plot the full height of the Hilo and Lihue sounding, rather than cutting them off at the height of Mauna Loa? Would these soundings look much different if you plotted them at full resolution?

In order to apply the TES H2O averaging kernel and a priori constraint to the Hilo and Lihue soundings I have to put them on the same grid as the TES estimate. In one of the original figures the full profile of each sounding was shown (without smoothing by the averaging kernel). However, these added figures made the plot even more busy than its current state. The full vertical profile of each sounding shows more vertical variability but the point of the comparison is to show how the sounding would appear if observed by TES. Clearly, the Hilo and Lihue soundings are quite different from the TES measurement, which is the point made in the manuscript and indicates why we cannot use nearby TES estimates for direct comparison. I have added additional language in Section 5.0 (along with the Barnes 2008 reference) emphasizing these points.

p. 78, ïňĄg 5: Could you show local time as well as UTC and mark with a vertical line the time of the TES overïňĆight? If the TES overïňĆight was at day 294.0, the corresponding in situ deltaD looks to be about -130, rather than the -180 shown in

ïňĄgure 3. ClariïňĄcation about this point (or just the vertical line showing the time of the TES overïňĆight) might be useful.

I have added the TES overpass time in these Figures as a vertical dashed line. You are correct about the -130 to -180 issue it is because of the large variance in H2O and delta-d for this day. I have added language in Section 5.1 discussing this variance. The large variance could also explain why the bias estimate from this comparison is different from the other 2 bias estimates.

p. 79, ïňĄg 6: What is the time resolution of the in situ data in ïňĄg 6? I am assuming that this is the raw in situ data and has not been processed into a TES estimate as in ïňĄg 3. Is this true?

The time resolution of the in situ data is so small (< 1 second?) that we have to average over a few seconds just to keep the data size manageable for file transfer over computers and consequently I have not kept track of this parameter. In addition, these in situ data are corrected using flasks and are averaged even further in time thereafter (Johnson reference). The time resolution does not matter for these comparisons because the variability over this time resolution is much smaller than the observed daily variations.

p. 81-88, ïňĄg A1-A8: I would encourage you to merge these ïňĄgures, pairing A1 and A5 into a single ïňĄgure, and so on.

I would like more time to think about presentation and ordering of these figures since I can come up with reasons to merge them or keep them separated. I will discuss with the editor once the paper is through the review process.

ïňĄg 5, A2 and A6: There are times in the HDO/H2O plots in each of these ïňĄgures (twice each day: near 293.6, 294.1, 295.8, 296.3, 309.7 and 310.2), where it appears that data is missing and the line connects the observations before and after this period. If the data is missing, do not plot anything at those times.

See response to earlier comment.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 25355, 2010.