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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 Response:

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.

Responses to Reviewer 1:

Major comments:

The two approaches rely on important assumptions. In my opinion a better documenta-

tion of these assumptions would be very useful. In the following I tried to collect all the assumption involved in method number one (constructing a "real profile" from surface observation):

I) The authors use the TES H2O profile data as a tracer in order to map the surface in-situ HDO/H2O to a HDO/H2O profile:

COMMENT: (1) Thereby the authors postulate that there is no bias between the TES H2O data and the in-situ H2O data. This is an important assumption and might cause important errors in the constructed "in-situ HDO/H2O profiles". In the current manuscript this assumption is not discussed at all.

RESPONSE: Bias in the lower tropospheric H2O data is less than 5% (Shepard et al., 2008) and in any case would not affect the distributions too much since the variability in H2O is much greater than the variability in delta-d. However, we have added the Shepard reference and indicated the expected bias in H2O in the manuscript.

COMMENT (2) Thereby the authors assume that the airmass in the middle/upper troposphere has the same history as the airmass at the Mauna Loa Observatory, page 25363, last line: "This mapping also makes the assumption that the observed air parcels measured over the day by the in situ device is representative of the observed air parcel measured at a single time by TES".

: I wonder if this is a realistic assumption for a subtropical site like Hawaii where large scale subsidence prevails. I could image that in regions with large scale subsidence the origins of lower/middle tropospheric air and middle/upper tropospheric air differ significantly.

RESPONSE: I agree with this assessment: As discussed in the revised error analysis section, we put very large errors on the middle / upper troposphere air that is not sampled by the in situ data (Section 5.3). However, as shown in the added error budget figures, lack of knowledge about these air parcels do not nullify our conclusions

because the sensitivity of the current TES measurements is small at these altitudes; they do affect our error estimates for the bias but we believe these error estimates are conservative due to the agreement in the bias estimates between measurements.

COMMENT: II) Bias correction (Equation 6): The authors only correct the bias for the retrieved HDO. However, an error in the line strength of HDO – as suspected by the authors (page 25366, line 13) – will also have an effect on the retrieved H2O. Instead of calculating the corrected ln[HDO] value the authors should calculate the corrected xr=ln[HDO]-ln[H2O] value: xr(corrected)= xr(original) – (ADD - AHD) * xD(bias) Only correcting HDO and then calculating the corrected HDO/H2O is to my understanding an assumption that might cause inconsistencies in the bias correction (ADD and AHD depend on the actual atmospheric situation like dry/wet conditions, clear/cloudy sky).

RESPONSE: We agree with this comment but do not see a way to distinguish the impact of uncertainties in the H2O spectroscopy from HDO spectroscopy on the ratio. Since the HDO vertical sensitivity is what determines the effective vertical sensitivity of the HDO/H2O estimate it is simplest to apply the bias correction via the HDO estimate. We have added a comment that additional validation needs to occur under wet conditions to better characterize the range of this bias correction.

COMMENT: III) Similar to item II): Equation (5) should consider that an error in the real HDO profile also propagates into the H2O profile. Equation (5) should be: STES = (ADD - AHD) * Sin-situ * (ADD - AHD)T

RESPONSE: The updated error analysis should include this effect as well as the effect of assuming that the TES H2O profile is the "true" profile. As discussed in the general comments errors in HDO and H2O are mitigated when constructing the ratio due to error cancellation (Section 5.0 Equation 4).

COMMENT IV) The "real" profile can only be deduced for pressures above 500 hPa. In the middle/upper troposphere (between 500 hPa and 200 hPa) it is determined by interpolating between the 500 hPa value and the a priori value at 200 hPa.

In my opinion there are a lot of important assumptions whose effects on the bias estimation are very difficult to assess. Therefore, I think the authors should be very cautious when drawing conclusions (maybe delete "very" on page 25369, line 11). It should be ensured that the reader gets the message that there remains an uncertainty in the bias of about (1-)2%. I suggest mentioning the assumptions already in the abstract, e.g., expand the last sentence of the abstract as follows: "... because these uncertainties are primarily derived from only three sets of measurements and rely on a variety of assumptions." RESPONSE: The updated error analysis shows a more conservative estimate of the errors ($\sim$1.9%). However, its also true that the bias estimates from the 3 measurements show differences that are much smaller than these errors which suggest that we are overestimating our errors. We indicate in the abstract that more comparisons are needed to refine the error in this bias estimate.

COMMENT: In addition, I suggest adding a Table that collects, documents, and discusses all the different assumptions that are made (for method one and two).

Response: While we can document the different error sources it is not easy to show that a particular error source contributes to XXX% an error on each measurement because of the changes in sensitivity and how the errors change when accounting for the TES sensitivity. Instead I have listed the different error terms in the error section (Section 5.3) and added a figure that shows their impact on the error budget.

The modeling community is already using the TES data and therefore, estimating the bias of TES – as done in the paper – is very urgent and important. In addition, the authors mention in the abstract that future studies are needed to refine this bias estimate. This is also my opinion:

COMMENT: In this context the authors mention another strategy that uses ground-based FTIR H2O and HDO/H2O profile observations as validation source (page 25358, lines 5ff). This would in my opinion be a better strategy. However, it is important to note that the bias in the ground-based FTIR data itself is not clearly documented (for

instance, Schneider et al., ACP, 6, 4705-4722, 2006; Schneider et al., AMT, 3, 1599-1613, 2010). It is planed to estimate the FTIR HDO/H2O bias during the next years by a variety of in-situ aircraft validation campaigns. FTIR data would then be best-suited for reviewing the TES bias estimation of this paper.

RESPONSE: Im looking forward to comparing the TES data with the FTIR data. We just need to get a post-doc working on this project!

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