

Authors' response to anonymous referee #1 on "Aircraft validation of Aura Tropospheric Emission Spectrometer retrievals of HDO and H₂O" by R. L. Herman et al., AMTD, 7, 3801-33, 2014.

We would like to thank the reviewer #1 for detailed review and helpful comments on our manuscript.

GENERAL COMMENTS:

Reviewer: "This paper describes the use of in situ observations of the HDO/H₂O ratio in water vapor to validate those made by TES. The approach of the analysis uses the fact that the in situ observations are precise and accurate enough to be considered the true values for atmospheric dD. The comparison of the in situ observations and the TES retrievals yields values for a bias error and an empirical error. Overall the paper is clear and well presented, with only a few exceptions listed below. The measurements are interesting and the paper will be a useful for those using TES data. There are a few comments and questions that I would like the authors to address."

Response: We have addressed all of the reviewer's specific comments and technical comments below.

SPECIFIC COMMENTS:

1a. Reviewer: "Why isn't the bias uncertainty included in the error budget? It is treated independently, but there is no reason given in the text for this treatment."

1a. Response: Referee #1 is absolutely correct that the TES bias uncertainty should be included in the error budget. We have revised Table 4 to reflect this.

1b. Reviewer: "Do you expect this bias to be the same everywhere for TES?"

1b. Response: This is an excellent point, also raised by the other reviewer. Within the error budget, we expect the bias to be the same everywhere because we attribute it to spectroscopy (see response 1d). To test our bias correction, we have reanalyzed TES – insitu δ D comparisons in two subtropical locations, Hawaii and the Mediterranean Sea. We compared TES version 5 observations with the Hawaii insitu data described by Worden et al. (2011), and with airborne Picarro measurements over the Mediterranean from the European HyMeX field mission (H. Sodemann, personal communication, 2014). Both sets of comparisons agree to within the TES estimated error, so we have confidence that the bias correction can be used globally. Our European collaborators requested that the HyMeX comparison not be shown in this paper (due to complications with the airborne instrument), so we have added the following brief text to the end of Section 4.3:

New Text on page 3813, line 5: "To test whether this bias correction can be applied globally, TES observations have been compared to coincident in situ measurements from Hawaii (Worden et al., 2011) and the Mediterranean Sea (H. Sodemann,

personal communication, 2014). Once the TES operator is applied to the in situ data (Eq. 1), the TES and in situ δD profiles agree to within the TES estimated error."

1c. Reviewer: "How do you justify the 20 per mil uncertainty on the bias?"

1c. Response: The 20 per mil uncertainty on the bias was estimated empirically by varying the prior by $\pm 30\text{‰}$ and seeing how much the bias changed (see page 3813, line 27, to page 3814, line 2).

1d. Reviewer: "The V004 bias was 63 per mil based on Mauna Loa data. Is this difference due to location? Retrieval? Changes in spectroscopy? Please explain and justify your approach."

1d. Response: The difference between the V004 bias and the V005 bias is due to changes in the retrieval: the V005 retrieval uses significantly more spectral lines than V004 (nearly the entire spectroscopic range from 1190 cm^{-1} to 1317 cm^{-1}), and V005 has a joint retrieval of the following four species: H_2O , HDO , N_2O and CH_4 . The new bias correction (Eq. 3) is consistent with the Hawaii data (see response 1b above). We infer that the bias is due to HDO spectroscopy. This is discussed in more detail by J. Worden et al., 2007, supplementary information and Worden et al. [2011]. We have new text to Section 4.3, page 3812, to explain this:

New text, page 3812, lines 14-15: "The source of this bias is inferred to be biases in spectroscopic line strengths of HDO , as discussed in the Supplementary Information of J. Worden et al. (2007)."

2. Reviewer: "As the paper is currently written you imply that after correcting for the 98 per mil bias, TES has a measurement error of ± 26 per mil in the BL. Unless you have a good reason, it seems to me that the uncertainty in the offset bias needs to be included in this number."

Response: We will add the uncertainty in the offset bias to Table 4 to be included in the error budget.

TECHNICAL COMMENTS:

1. Reviewer: "Title: The paper does not really discuss the validation of HDO and H_2O independently, only the ratio. I suggest a title using δD or the ratio $\text{HDO}/\text{H}_2\text{O}$ in the title."

Response: The reviewer has a good point. We will change the title of this paper to
New text: "Aircraft validation of Aura Tropospheric Emission Spectrometer retrievals of $\text{HDO}/\text{H}_2\text{O}$ "

2. Reviewer: "Abstract: Use the per mil units for the bias errors. Also a few places in the text need to be changed. (pg 13, 16)"

Response: We will change the abstract and pages 13,16 to per mil notation:
Page 3802, lines 19-21 changed to, "...approximately +123‰ at 1000 hPa, +98‰ in the boundary layer, and +37‰ in the free troposphere. The uncertainty in this bias estimate is $\pm 20\%$."

Page 3807, line 5, changed to, "... TES V004 δD data are biased high by $+63 \pm 19\%$.
Page 3813, lines 3-5 changed to, "This corresponds to a typical TES bias of +98‰ in the boundary layer (average of 909 and 825 hPa pressure levels), and +37‰ in the free troposphere (average of eight pressure levels between 750 and 383 hPa)."
Page 3816, lines 7-9 changed to, "This amounts to a net bias correction of -98‰ in the boundary layer, gradually reduced to -37‰ in the free troposphere. The uncertainty in the bias correction is estimated to be $\pm 20\%$."

3. Reviewer: "pg 11, line 14. Why are the 1000 hPa levels excluded?"

Response: The 1000 hPa pressure level is excluded because TES has less sensitivity at the surface than at 909 hPa level (corresponding to 900 m aircraft altitude). Furthermore, some of the inland Alaska geolocations are elevated terrain with surface pressures much less than 1000 hPa. We begin the comparison at 909 hPa.

4. Reviewer: "Page 11, Eq. 1, and Figure 3b: I am curious how this TES operator works with in situ data. I went to the Worden 2006 JGR reference and did not find a good explanation (none at all, really). Can you provide a better reference or explain in the text? This had a large effect on dD in the BL (+50 per mil), so it is important for the reader to understand."

Response: The reviewer has a good point here. Two key references are missing from the discussion (H. Worden et al., 2007; and Herman and Kulawik, 2014), so I have added them. We have added further text to section 3.3 (page 3809) to better explain the method of comparison:

New Text on page 3809:

"3.3 Method of comparison"

Following the approach of Rodgers and Connor (2003), satellite and *in situ* data may be compared directly if the satellite averaging kernel is applied to the *in situ* data to treat both atmospheric profiles with the same vertical sensitivity. Aircraft *in situ* measurements have a much finer vertical resolution than satellite retrievals. The TES operator, which consists of the *a priori* constraint vector x_a and the TES averaging kernel matrix A , is used to smooth the *in situ* data to the same resolution as the satellite retrievals. The averaging kernel matrix A is the sensitivity of the TES estimate to the true concentration in the atmosphere (Rodgers, 2000). TES retrievals are performed on the logarithm of the volume mixing ratios, $x_D = \ln(q_D)$ and $x_H = \ln(q_H)$. H. Worden et al. (2007) have described in detail how the TES operator is applied to *in situ* measurements of ozone.

For comparisons of HDO/H₂O, the state vectors for HDO and H₂O are stacked together, so that the first half levels are HDO and the second half levels are H₂O, as described in Worden et al. (2006), Eq. (3), and in the Lite Products Appendix of the TES L2 Data

Users' Guide (Herman and Kulawik, 2014). Worden et al. (2006) denotes \hat{x} as the TES estimate of HDO and H₂O, x as the true state of HDO and H₂O, and the averaging kernel for the ratio as:

$$A_{xx} = \begin{pmatrix} A_{DD} & A_{DH} \\ A_{HD} & A_{HH} \end{pmatrix}$$

where $A_{DH} = \frac{\partial \hat{x}_D}{\partial x_H}$, the derivative of the HDO estimate with respect to the true state of H₂O, and other blocks of the matrix are defined similarly.

For comparison with TES, the in situ HDO and H₂O profiles are extended to cover the full range of TES levels. In the boundary layer, from the surface up to the lowest altitude aircraft data, we assume constant values of HDO and H₂O set equal to the first aircraft measurement. In the range of aircraft data (boundary layer to aircraft ceiling), the aircraft in situ HDO and H₂O data are interpolated to the levels of the TES forward model. It is quite likely that fine scale features are not captured this way, but these features are negligible at the TES vertical resolution (see averaging kernel in Fig. 3c). In the top layer, above the aircraft maximum altitude, the profile is extrapolated using a scaled *a priori* profile (see Sect. 4.4 for details). Next, $x_{insitu/AK}$ is calculated jointly for HDO and H₂O using the TES operator:

$$x_{insitu/AK} = x_a + A_{xx}(x - x_a) \quad (1)$$

where $x_{insitu/AK}$ is the *in situ* profile with applied averaging kernel and *a priori* constraint. In this paper, all comparisons have been completed using the TES operator."

5. Reviewer: "Page 12: and Figure 4. This is really the TES measurement corrected for the bias. The thin black lines are TES_corrected_for_bias – insitu. The thick black line is then the residual bias after the bias correction? It would be helpful for you to explicitly identify all TES measurements in the figures as having been corrected for the bias somehow. Here you could explain much more about the bias and what you think the source is. Is it spectroscopic? Do you expect it to be constant for all retrievals everywhere?"

Response: We have addressed this point in the specific comments 1b and 1d above. The source of the bias is inferred to be HDO spectroscopy.

The referee is correct that in Figure 4 and other figures, TES is corrected for the bias. We have added a figure 4a (the bias), 4b (TES minus aircraft, no bias correction), and 4c (bias-corrected TES minus aircraft). We changed the figure 4c caption to read:

"Fig. 4c. Comparisons of TES δD corrected for bias minus aircraft δD , with averaging kernel applied for the 16 scans that have good quality, DOFS>1.1, and spatially overlap the aircraft flight path (see Table 1). Also plotted are the TES residual bias after bias correction (thick black line) and standard deviation (dashed red line). In this figure TES HDO has been corrected by δ_{bias} (Eq. 3)."

6. Reviewer: “page 13 lines 15 – 20 are confusing. Do you subtract a constant or multiply by a constant?”

Response: The scaling mentioned here is multiplication by a constant. We have replaced the text on page 3813, lines 15 to 20, with:

New text, page 3813, lines 15-20:

“The prior HDO/H₂O profile is multiplied by a constant factor so that its value at the TES level nearest the aircraft ceiling matches the aircraft HDO/H₂O. The prior HDO/H₂O is multiplied by the same constant factor at levels from the aircraft ceiling up to the tropopause. An unscaled prior is used above the tropopause.”

7. Reviewer: “Page 16 line 20. You should state that these empirical errors are after applying the correction for the bias of 98 and 37 per mil.”

Response: The referee is correct. We have changed the text to:

New text on page 3816, lines 19-22: “From matched TES-aircraft pairs of observations, we estimate the TES empirical error ($1-\sigma$ st. dev.). After bias correction, the TES empirical error is $\pm 26\%$ in the boundary layer, and $\pm 22\%$ in the free troposphere below the ceiling of the aircraft measurements (see Sect. 5).”

8. Reviewer: “All figures please use a) b) etc instead of left and right. Several labels are hard to read, especially Fig 3 labels. Also, thick lines could be thicker. They are hard to read in reduced sizes.”

Response: We have taken the referee’s suggestions to improve all figures with labels of a,b instead of left/right, larger labels, and thicker lines.