Supplement to: **Comparison of Optimal Estimation HDO/H_2O Retrievals from AIRS with ORACLES measurements**

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Sensitivity of retrievals to the choice of forward model

In this supplement we assess the sensitivity of HDO and H_2O retrievals to the choice of forward model. All the retrievals in this paper were obtained from the MUSES retrieval framework using the Optimal Spectral Sampling (OSS) forward model (Moncet et al., 2008, 2015). The OSS method was designed specifically for the modeling of radiances measured by sounding radiometers in the infrared (Moncet et al., 2008, 2015), although it is applicable throughout the microwave, visible, and ultraviolet spectral regions. OSS uses an extension of the exponential sum fitting of transmittances technique in that channel-average radiative transfer is obtained from a weighted sum of monochromatic calculations. Among the advantages of the OSS method is that its numerical accuracy, with respect to a reference line-by-line model, is selectable, allowing the model to provide whatever balance of accuracy and computational speed is optimal for a particular application. Only a few monochromatic points are required to model channel radiances with a brightness temperature accuracy of 0.05 K. The version of OSS used here is trained with the monochromatic Atmospheric and Environmental Research, Inc. (AER) Line-By-Line Radiative Transfer Model (LBLRTM_v12.4) (Clough et al., 2005) using spectroscopic parameters from the 'HIgh-resolution TRANsmission' database (HITRAN12) (Rothman et al., 2013) plus line coupling coefficients for CO_2 and CH_4 calculated at AER.

Historically, retrievals from the TES instrument were carried out using the operational 'Earth Limb and Nadir Operational Retrieval' (ELANOR) code as a forward model (Clough et al., 2006). ELANOR incorporates most of the physics contained in LBLRTM, but rather than calculating molecular optical depths line-by-line, it uses pre-calculated look-up tables of absorption coefficients indexed by species, pressure and temperature. The coefficients in this table were generated by running LBLRTM_v12.4 with the same line file as used for OSS. Since ELANOR runs calculations on a fine spectral grid, and the timing for calculations scales according to the number of spectral points, it is an order of magnitude slower than OSS. This was the main motivation for switching to OSS for MUSES in general and these AIRS retrievals in particular.

Both OSS and ELANOR have been extensively validated against results from LBLRTM. However, there are some differences in the details of implementation. For example, ELANOR treats the HDO as a completely separate molecule from the main water isotopologue, whereas OSS treats HDO in terms of a ratio to the main isotopologue. This leads to some differences in the water vapor Jacobians. In addition, there are some minor differences in the implementation of the cloud optical depth Jacobians. In order to provide some insight into the impact of differences between the two models, the retrievals from AIRS during a single day of the ORACLES campaign (August 31, 2016) were run using both models and the differences between the models were compared to the AIRS minus WISPER differences (Figure S1). Percent differences between A and B are calculated as 100*(A-B)/[0.5*(A+B)].

The H_2O results (Figure S1, top panels) show that between the surface and 4 km altitude OSS retrievals are biased low compared to the WISPER data, while ELANOR retrievals are biased low compared to OSS retrievals; therefore OSS H_2O retrievals appear more accurate. The HDO results (Figure 1, bottom panels) show that the AIRS OSS retrievals were on average unbiased at the surface and at 3.5 km, and presented a small negative bias between those altitudes, which peaked around 2 km. ELANOR retrievals are biased high with respect to OSS retrievals over this range, especially between the surface and 2 km, which implies that HDO from ELANOR is too high at the surface but agrees better with the WISPER data with increasing altitude up to 3.5 km. Above this altitude ELANOR retrievals are biased low with respect to OSS retrievals, and therefore present a larger negative bias with respect to WISPER than the OSS retrievals do. Overall, the OSS results agree better with the WISPER data than the ELANOR retrievals.

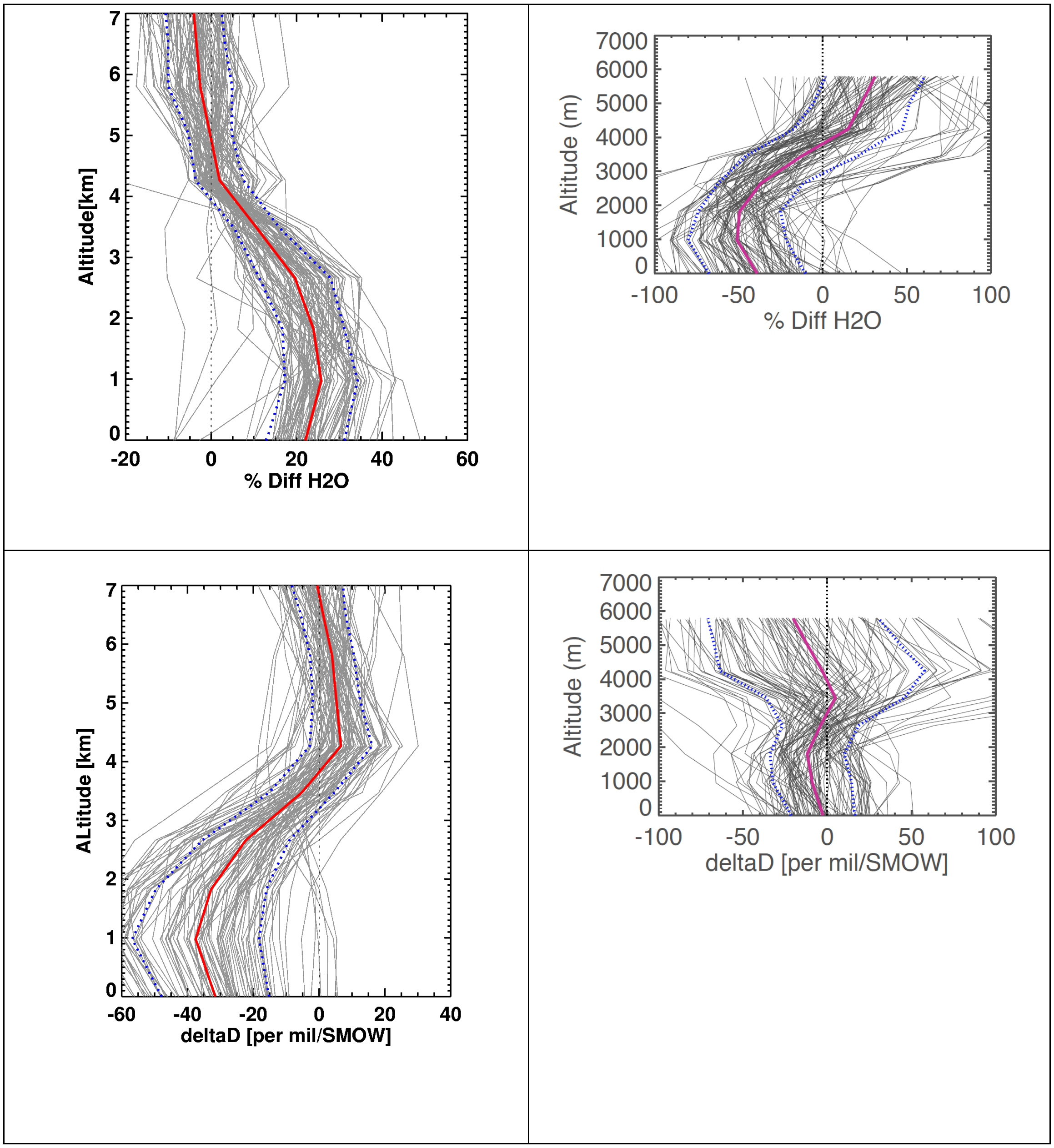

Figure S1. AIRS OSS H_2O (top) and Delta-D (bottom) biases with respect to ELANOR retrievals (left) and WISPER data (right). Lines are individual profiles (black lines), mean (red solid line) and mean ± RMS (dotted blue lines).

Code/Data availability. The ORACLES aircraft data used in the data analysis can be freely downloaded from the following Digital Object Identifier: (http://dx.doi.org/10.5067/Suborbital/ORACLES/P3/2016_V1, last access: 22 April 2017). We expect the AIRS-based deuterium data to be publicly released by January 2020. Files in IDL format of the AIRS data shown and forward model output are available from coauthor John Worden upon request: john.r.worden@jpl.nasa.gov.

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Author contribution. RH carried out all steps of aircraft validation, from matching data and quality filtering to applying observation operator and statistics, while JW provided satellite-to-satellite validation. JW developed the retrieval strategies for both AIRS and TES HDO/H_2O retrievals. DF and SK built the strategies of single AIRS footprint HDO/H_2O retrievals into the MUSES algorithm. KC, RH and VP evaluated the sensitivities of retrievals to the choice of forward model. RH, VP, JW, SK, DF, DN, DH and KB contributed to the text and interpretation of the results. JW and SK helped in the estimation of HDO/H_2O measurement uncertainty, quality flagging and knowledge of the retrieval process. DN and DH provided ORACLES data, aircraft measurement uncertainty, and identified profiles in the aircraft data. All authors participated in writing the manuscript.

Competing interests. The authors declare that they have no conflict of interest.

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References in the Supplement

Clough, S. A., Shephard, M. W., Mlawer, E. J., Delamere, J. S., Iacono, M. J., Cady-Pereira, K., Boukabara, S., and Brown, R.D.: Atmospheric radiative transfer modeling: a summary of the AER codes, J. Quant. Spectrosc. Radiat. Transfer, 91, 233–244, 2005.

Clough, S. A., Shephard, M. W., Worden, J., Brown, P. D., Worden, H. M., Luo, M., Rodgers, C. D., Rinsland, C. P., Goldman, A., Brown, L., Kulawik, S. S., Eldering, A., Lampel, M., Osterman, G., Beer, R., Bowman, K., Cady-Pereira, K. E., Mlawer, E. J.: IEEE Transac. Geosci. Rem. Sens., 44(5), 1308-1323, 2006.

Moncet, J. L., Uymin, G., Lipton, A. E., and Snell, H. E.: Infrared radiance modeling by optimal spectral sampling, J. Atmos. Sci., 65, 3917–3934, 2008.

Rothman, L. S., Gordon, I. E., Babikov, Y., Barbe, A., Chris Benner, D., Bernath, P. F., Birk, M., Bizzocchi, L., Boudon, V., Brown, L. R., Campargue, A., Chance, K., Cohen,

E. A., Coudert, L. H., Devi, V. M., Drouin, B. J., Fayt, A., Flaud, J.-M., Gamache, R. R., Harrison, J. J., Hartmann, J.-M., Hill, C., Hodges, J. T., Jacquemart, D., Jolly, A., Lamouroux, J., Le Roy, R. J., Li, G., Long, D. A., Lyulin, O. M., Mackie, C. J., Massie, S. T., Mikhailenko, S., Müller, H. S. P., Naumenko, O. V., Nikitin, A. V., Orphal, J., Perevalov, V., Perrin, A., Polovtseva, E. R., Richard, C., Smith, M. A. H., Starikova, E., Sung, K., Tashkun, S., Tennyson, J., Toon, G. C., Tyuterev, V. G., and Wagner, G.: The HITRAN2012 molecular spectroscopic database, J. Quant. Spectrosc. Radiat. Transfer, 130, 4–50, 2013.