

Supplement of Atmos. Meas. Tech., 13, 1825–1834, 2020
<https://doi.org/10.5194/amt-13-1825-2020-supplement>
© Author(s) 2020. This work is distributed under
the Creative Commons Attribution 4.0 License.



Supplement of

Comparison of optimal estimation HDO/H₂O retrievals from AIRS with ORACLES measurements

Robert L. Herman et al.

Correspondence to: Robert L. Herman (robert.l.herman@jpl.nasa.gov)

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.

17 **Sensitivity of retrievals to the choice of forward model**

18 In this supplement we assess the sensitivity of HDO and H₂O retrievals to the choice of
19 forward model. All the retrievals in this paper were obtained from the MUSES retrieval
20 framework using the Optimal Spectral Sampling (OSS) forward model (Moncet et al.,
21 2008, 2015). The OSS method was designed specifically for the modeling of radiances
22 measured by sounding radiometers in the infrared (Moncet et al., 2008, 2015), although it
23 is applicable throughout the microwave, visible, and ultraviolet spectral regions. OSS
24 uses an extension of the exponential sum fitting of transmittances technique in that
25 channel-average radiative transfer is obtained from a weighted sum of monochromatic
26 calculations. Among the advantages of the OSS method is that its numerical accuracy,
27 with respect to a reference line-by-line model, is selectable, allowing the model to
28 provide whatever balance of accuracy and computational speed is optimal for a particular
29 application. Only a few monochromatic points are required to model channel radiances
30 with a brightness temperature accuracy of 0.05 K. The version of OSS used here is
31 trained with the monochromatic Atmospheric and Environmental Research, Inc. (AER)
32 Line-By-Line Radiative Transfer Model (LBLRTM_v12.4) (Clough et al., 2005) using
33 spectroscopic parameters from the ‘High-resolution TRANsmision’ database
34 (HITRAN12) (Rothman et al., 2013) plus line coupling coefficients for CO₂ and CH₄
35 calculated at AER.

36

37 Historically, retrievals from the TES instrument were carried out using the operational
38 ‘Earth Limb and Nadir Operational Retrieval’ (ELANOR) code as a forward model
39 (Clough et al., 2006). ELANOR incorporates most of the physics contained in LBLRTM,

40 but rather than calculating molecular optical depths line-by-line, it uses pre-calculated
41 look-up tables of absorption coefficients indexed by species, pressure and temperature.
42 The coefficients in this table were generated by running LBLRTM_v12.4 with the same
43 line file as used for OSS. Since ELANOR runs calculations on a fine spectral grid, and
44 the timing for calculations scales according to the number of spectral points, it is an order
45 of magnitude slower than OSS. This was the main motivation for switching to OSS for
46 MUSES in general and these AIRS retrievals in particular.

47

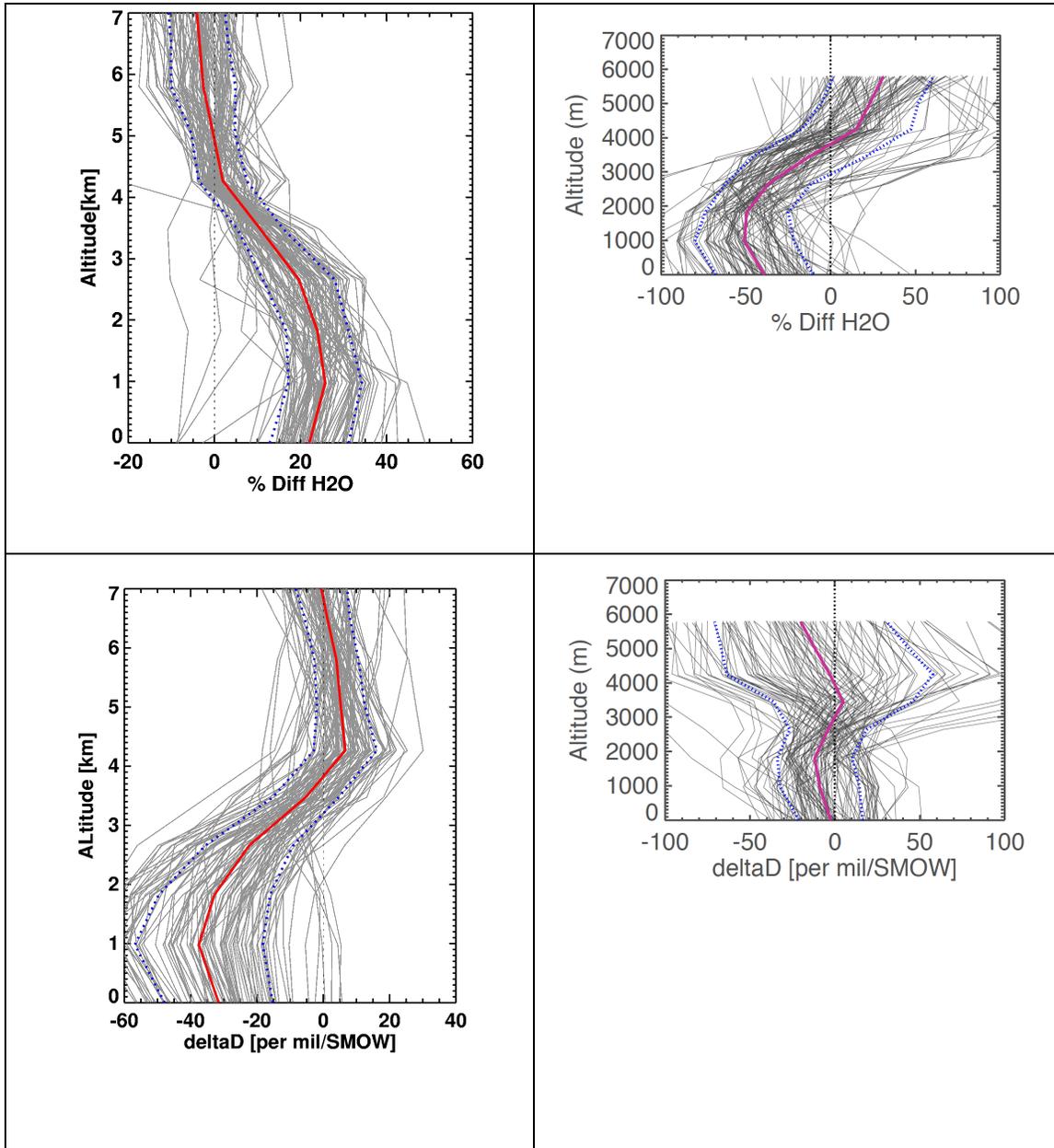
48 Both OSS and ELANOR have been extensively validated against results from LBLRTM.
49 However, there are some differences in the details of implementation. For example,
50 ELANOR treats the HDO as a completely separate molecule from the main water
51 isotopologue, whereas OSS treats HDO in terms of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

59

60 The H₂O results (Figure S1, top panels) show that between the surface and 4 km altitude
61 OSS retrievals are biased low compared to the WISPER data, while ELANOR retrievals
62 are biased low compared to OSS retrievals; therefore OSS H₂O retrievals appear more

63 accurate. The HDO results (Figure 1, bottom panels) show that the AIRS OSS retrievals
64 were on average unbiased at the surface and at 3.5 km, and presented a small negative
65 bias between those altitudes, which peaked around 2 km. ELANOR retrievals are biased
66 high with respect to OSS retrievals over this range, especially between the surface and 2
67 km, which implies that HDO from ELANOR is too high at the surface but agrees better
68 with the WISPER data with increasing altitude up to 3.5 km. Above this altitude
69 ELANOR retrievals are biased low with respect to OSS retrievals, and therefore present a
70 larger negative bias with respect to WISPER than the OSS retrievals do. Overall, the OSS
71 results agree better with the WISPER data than the ELANOR retrievals.

72



73

74 **Figure S1.** AIRS OSS H₂O (top) and Delta-D (bottom) biases with respect to ELANOR
 75 retrievals (left) and WISPER data (right). Lines are individual profiles (black lines), mean
 76 (red solid line) and mean \pm RMS (dotted blue lines).

77

78

79 **Code/Data availability.** The ORACLES aircraft data used in the data analysis can be
80 freely downloaded from the following Digital Object Identifier:
81 (http://dx.doi.org/10.5067/Suborbital/ORACLES/P3/2016_V1, last access: 22 April
82 2017). We expect the AIRS-based deuterium data to be publicly released by January
83 2020. Files in IDL format of the AIRS data shown and forward model output are
84 available from coauthor John Worden upon request: john.r.worden@jpl.nasa.gov.

85
86 **Team list.** Robert L. Herman (RH), John Worden (JW), David Noone (DN), Dean
87 Henze (DH), Kevin Bowman (KB), Karen Cady-Pereira (KC), Vivienne H. Payne (VP),
88 Susan S. Kulawik (SK), and Dejian Fu (DF).

89
90 **Author contribution.** RH carried out all steps of aircraft validation, from matching data
91 and quality filtering to applying observation operator and statistics, while JW provided
92 satellite-to-satellite validation. JW developed the retrieval strategies for both AIRS and
93 TES HDO/H₂O retrievals. DF and SK built the strategies of single AIRS footprint
94 HDO/H₂O retrievals into the MUSES algorithm. KC, RH and VP evaluated the
95 sensitivities of retrievals to the choice of forward model. RH, VP, JW, SK, DF, DN, DH
96 and KB contributed to the text and interpretation of the results. JW and SK helped in the
97 estimation of HDO/H₂O measurement uncertainty, quality flagging and knowledge of the
98 retrieval process. DN and DH provided ORACLES data, aircraft measurement
99 uncertainty, and identified profiles in the aircraft data. All authors participated in writing
100 the manuscript.

101

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

103

104 **Acknowledgements**

105 Part of the research described in this paper was carried out by the Jet Propulsion
106 Laboratory, California Institute of Technology, under a contract with NASA.

107

108

109 **References in the Supplement**

110

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

114

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

119

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

122

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

125 E. A., Coudert, L. H., Devi, V. M., Drouin, B. J., Fayt, A., Flaud, J.-M., Gamache, R. R.,
126 Harrison, J. J., Hartmann, J.-M., Hill, C., Hodges, J. T., Jacquemart, D., Jolly, A.,
127 Lamouroux, J., Le Roy, R. J., Li, G., Long, D. A., Lyulin, O. M., Mackie, C. J., Massie,
128 S. T., Mikhailenko, S., Müller, H. S. P., Naumenko, O. V., Nikitin, A. V., Orphal, J.,
129 Perevalov, V., Perrin, A., Polovtseva, E. R., Richard, C., Smith, M. A. H., Starikova, E.,
130 Sung, K., Tashkun, S., Tennyson, J., Toon, G. C., Tyuterev, V. G., and Wagner, G.: The
131 HITRAN2012 molecular spectroscopic database, *J. Quant. Spectrosc. Radiat. Transfer*,
132 130, 4–50, 2013.