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3 **Comparison of Optimal Estimation HDO/H<sub>2</sub>O Retrievals**  
4 **from AIRS with ORACLES measurements**

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16



17 **Abstract**

18 In this paper we evaluate new retrievals of the deuterium content of water vapor from the  
19 Aqua Atmospheric InfraRed Sounder (AIRS) with aircraft measurements of HDO and  
20 H<sub>2</sub>O from the ObseRvations of Aerosols above Clouds and their intEractionS  
21 (ORACLES) field mission. Single footprint AIRS radiances are processed with an  
22 optimal estimation algorithm that provides a vertical profile of the HDO/H<sub>2</sub>O ratio,  
23 characterized uncertainties, and instrument operators (or averaging kernel matrix). These  
24 retrievals are compared to vertical profiles of the HDO/H<sub>2</sub>O from the Oregon State  
25 University Water Isotope Spectrometer for Precipitation and Entrainment Research  
26 (WISPER) on the ORACLES NASA P-3B Orion aircraft. Measurements were taken over  
27 the Southeast Atlantic Ocean from 31 August to 25 September 2016. HDO/H<sub>2</sub>O is  
28 commonly reported in  $\delta D$  notation, which is the fractional deviation of the HDO/H<sub>2</sub>O  
29 ratio from the standard reference ratio. For collocated measurements, the satellite  
30 instrument operator (averaging kernels and a priori constraint) is applied to the aircraft  
31 profile measurements. We find that AIRS  $\delta D$  bias relative to the aircraft is well within  
32 the estimated measurement uncertainty. In the lower troposphere, 1000 to 800 hPa, AIRS  
33  $\delta D$  bias is -6.6‰ and the Root Mean Square (RMS) deviation is 20.9‰, consistent with  
34 the calculated uncertainty of 19.1‰. In the mid-troposphere, 800 to 500 hPa, AIRS  $\delta D$   
35 bias is -6.8‰ and RMS 44.9‰, comparable to the calculated uncertainty of 25.8‰.



36 **1. Introduction**

37 The deuterium content of tropospheric water vapor is sensitive to the different types of  
38 atmospheric moisture sources such as evaporation from the ocean or land and the  
39 processing that occurs during transport such as mixing or condensation (e.g., Craig, 1961;  
40 Dansgaard, 1964; Galewsky et al., 2016). Condensation and precipitation preferentially  
41 remove the heavier HDO isotopologue from the gas phase relative to the parent  
42 isotopologue H<sub>2</sub>O, whereas evaporation of precipitation at lower altitudes in the  
43 atmosphere can enrich HDO relative to H<sub>2</sub>O vapor. These unique, isotopic properties  
44 allow HDO/H<sub>2</sub>O to be a tracer for the origin, condensation and evaporation history of an  
45 air parcel, thus useful for evaluating changes to the water cycle (e.g., Worden et al., 2007;  
46 Noone, 2012; Galewsky et al., 2016).

47

48 In the last decade, satellite retrievals of the isotopic composition of tropospheric water  
49 vapor (HDO and H<sub>2</sub>O) have been developed, including Envisat/SCIAMACHY (Scanning  
50 Imaging Absorption Spectrometer for Atmospheric Chartography) (Frankenberg et al.,  
51 2009), IASI (Infrared Atmospheric Sounding Interferometer) aboard the MetOp satellites  
52 (Herbin et al., 2009; Schneider and Hase, 2011; Lacour et al., 2012), and TES (the  
53 Tropospheric Emission Spectrometer) on the Aura spacecraft (Worden et al., 2006;  
54 Worden et al., 2007). More recently, Worden et al. have developed HDO retrievals from  
55 the Aqua Atmospheric InfraRed Sounder (AIRS) single footprint Level 1b radiance data  
56 (Worden et al., 2019). These AIRS retrievals are the subject of the present comparison  
57 with aircraft data.

58



59 Satellite HDO measurements have been utilized to study tropical carbon/water feedbacks  
60 (Wright et al., 2017), moist processes in deep convection (e.g. Worden et al., 2007), and  
61 the global partitioning of transpiration to evapotranspiration (Good et al., 2015). A  
62 decadal record of HDO has promise in characterizing global shifts in moisture sources  
63 and atmospheric water balance in response to warming, climactic variability, and land-  
64 use. For example, Bailey et al. (2017) shows that a record of free-tropospheric HDO/H<sub>2</sub>O  
65 would provide an observational constraint on changes in the tropical water balance  
66 (evaporation minus precipitation) in response to shifts in ocean temperature. Wright et al.  
67 (2017) also shows that free-tropospheric deuterium measurements provide a fundamental  
68 new constraint in carbon / water dynamics in the Amazon. They use the TES isotope  
69 measurements to show that dry-season evapotranspiration is critical towards initiating the  
70 southern Amazon rainfall, which in turn is critical towards sustaining the Amazon  
71 rainforest (Fu et al., 2013). For these reasons a record of the deuterium content of water  
72 vapor from the long (17 years and continuing) record from AIRS holds significant  
73 potential to evaluate changes in the global water cycle.

74

75 This paper presents detailed comparisons between new AIRS measurements of the  
76 deuterium content of water vapor (or HDO/H<sub>2</sub>O ratio) and accurate *in situ* HDO/H<sub>2</sub>O  
77 measurements from an aircraft sensor during the NASA ObseRvations of Aerosols above  
78 Clouds and their intEractionS (ORACLES) field mission. In this paper, we denote the  
79 volume mixing ratios  $q_D$  for HDO, and  $q_H$  for H<sub>2</sub>O. By standard convention, we report  
80 the isotopic abundance as  $\delta D$  (per mil or ‰) =  $[(q_D/q_H)_{obs}/(q_D/q_H)_{std} - 1] * 1000$ ,



81 where  $(q_D/q_H)_{std} = 3.11 \times 10^{-4}$  based on the D/H standard ratio for Vienna Standard Mean  
82 Ocean Water (SMOW).

83

## 84 **2. Instrumentation**

### 85 **2.1 AIRS Instrument Description**

86 The Atmospheric InfraRed Sounder (AIRS) on the NASA Aqua satellite is a nadir-  
87 viewing, scanning thermal infrared grating spectrometer that covers the 3.7 to 15.4  $\mu\text{m}$   
88 spectral range with 2378 spectral channels (Pagano et al., 2003, and Aumann et al.,  
89 2003). Launched on May 4, 2002, Aqua is in a sun-synchronous orbit at 705 km with an  
90 approximately 1:30 pm equator crossing-time as part of the A-Train satellite  
91 constellation. AIRS continues to make daily measurements of most of the globe with its  
92 wide cross-scanning swath of coverage. The AIRS instrument makes collocated  
93 measurements with the Advanced Microwave Sounding Unit (AMSU) on the Aqua  
94 satellite. There are nine AIRS single footprint observations (nadir horizontal resolution of  
95  $\sim 13.5$  km) arranged in a 3 by 3 grid within a single AMSU footprint of  $\sim 45$  km (Aumann  
96 et al., 2003). For HDO retrievals, the single footprint AIRS Level 1b (L1b) radiances are  
97 utilized. Absolute radiometric accuracy between 220 K and 320 K at all observation  
98 angles is better than 0.2 K (Pagano et al., 2003, 2008). The algorithm applied to AIRS  
99 radiances to yield HDO is described below in Sect. 3.1.

100

### 101 **2.2 WISPER system for aircraft measurements**

102 Aircraft measurements were made on the NASA P-3B Orion aircraft during the NASA  
103 ORACLES field mission. ORACLES is a five-year Earth Venture Suborbital (EVS-2)



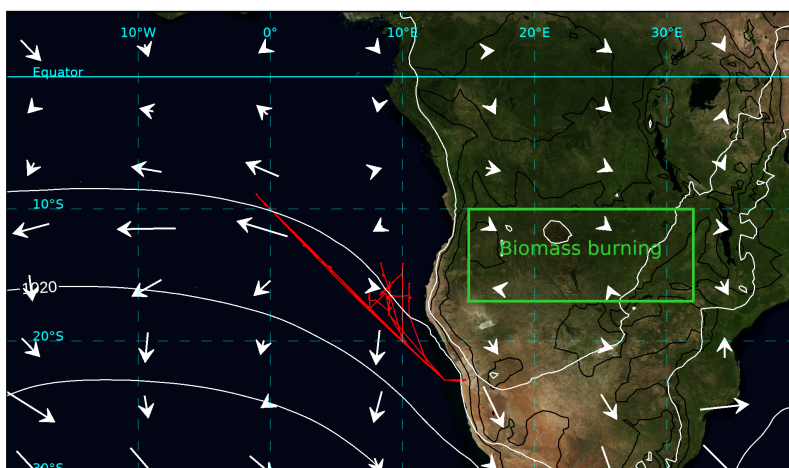
104 investigation with three Intensive Observation Periods (IOP) designed to study key  
105 processes that determine the climate impacts of African biomass burning aerosols in  
106 2016, 2017, and 2018. The ORACLES experiment provided multi-year airborne  
107 observations from the NASA P-3B Orion and ER-2 aircraft over the complete vertical  
108 column of the key parameters that drive aerosol-cloud interactions in the southeast  
109 Atlantic Ocean region. The focus of the ORACLES field measurements was a biomass  
110 burning plume that advected west from the African continent to the lower troposphere (at  
111 2 to 5 km above sea level, ASL) above the Atlantic Ocean. Here we use data from the  
112 ORACLES 2016 IOP (ORACLES Science Team, 2017), and report on aircraft versus  
113 satellite comparisons from eight flights (Fig. 1 and Table 1).

114

115 Water vapor isotopic abundances ( $\text{HDO}/\text{H}_2\text{O}$  and  $\text{H}_2^{18}\text{O}/\text{H}_2^{16}\text{O}$ ) were measured in situ on  
116 the aircraft with the Oregon State Water WISPER system (Water Isotope Spectrometer  
117 for Precipitation and Entrainment Research, Henze et al., in prep.), which uses a modified  
118 commercial Picarro L2120-i  $\delta\text{D}/\delta^{18}\text{O}$  Ultra High-Precision Isotopic Water Analyzer. The  
119 measurement technique is cavity ring-down (CRD) spectroscopy (O'Keefe and Deacon,  
120 1988; Berden et al., 2000; Gupta et al., 2009). The majority of measurements analyzed in  
121 this paper are located within the biomass burning plume, characterized by elevated  $\text{H}_2\text{O}$   
122 (approximately 6000 ppmv) and elevated  $\delta\text{D}$  (-100 to -70‰). At these abundances of  
123  $\text{HDO}/\text{H}_2\text{O}$ , the 1-Hz precision ( $1\sigma$ ) of the measurements of  $\delta\text{D}$  is  $\pm 3\%$ , and the accuracy  
124 is  $\pm 6.5\%$ .

125

126



127

128 **Figure 1.** Selected flight tracks (red lines) of the NASA P-3B Orion aircraft during the  
129 ORACLES 2016 IOP used in this study, with corresponding flight dates listed in Table 1.

130 Also shown is the biomass burning region (green rectangle), 700 hPa winds (white  
131 vectors), and surface pressure (white isobars).

132

133 **Table 1.** Summary of matches AIRS and WISPER  $\delta D$  measurements during NASA ORACLES\*.

Flight Date	Daily Number of Matched Profiles, loose lat/lon constraint.	Daily Number of Matched Profiles, tighter lat/lon constraint.
31-Aug-2016	138	26
2 Sep 2016	15	15



4 Sep 2016	102	26
10 Sep 2016	48	7
12 Sep 2016	18	4
14 Sep 2016	12	5
20 Sep 2016	11	4
25 Sep 2016	102	23
<b>Total</b>	<b>446</b>	<b>110</b>

134 \*NASA ORACLES is the “ObseRvations of Aerosols above Clouds and their intEractionS” Earth Venture  
135 Suborbital Mission.  
136

### 137 **3 Satellite Retrieval**

#### 138 **3.1 Retrieval Algorithm**

139 The single footprint AIRS HDO profile data used in this work were produced using the  
140 retrieval algorithm, named the MUlTi-SpEctra, MUlTi-SpEcies, MUlTi-Sensors (MUSES)  
141 algorithm (Fu et al., 2013, 2016, 2018; Worden et al., 2019). The MUSES algorithm can  
142 use radiances from multiple instruments including AIRS and other instruments (CrIS,  
143 TES, OMI, OMPS, TROPOMI, and MLS) to quantify geophysical observables that affect  
144 the corresponding radiance. The AIRS single footprint HDO profile retrievals have been  
145 described by Worden et al. (2019), and have heritage from the TES algorithm (Worden et  
146 al., 2004, 2006, 2007, 2011, 2012, 2013; Bowman et al. 2006, 2002). The Optimal  
147 Spectral Sampling (OSS) fast radiative transfer model (Moncet et al., 2008, 2015) for  
148 single footprint AIRS measurements has been integrated into the MUSES algorithm, in  
149 support of the operational data production towards the multi-decadal record of global  
150 HDO profiles. The supplement attached to this paper discusses the sensitivity of the  
151 retrievals to the choice of forward model. The retrieval uses the optimal estimation  
152 method to quantify atmospheric HDO and H<sub>2</sub>O (Worden et al. 2006, 2012, 2019). For





153 both AIRS and TES retrievals, height discrimination of the HDO/H<sub>2</sub>O ratio in the  
154 troposphere is provided by spectral resolution of pressure and temperature broadened  
155 absorption features of their corresponding lines (Beer et al., 2002). The algorithms and  
156 spectral microwindows are described by Worden et al. (2019). Chemical species CH<sub>4</sub>,  
157 CO, HDO, and H<sub>2</sub>O are jointly retrieved along with atmospheric temperature, surface  
158 temperature, land emissivity and clouds (Worden et al. 2012). The retrieval optimizes the  
159 ratio of HDO to H<sub>2</sub>O, as opposed to either HDO or H<sub>2</sub>O alone (Worden et al., 2019,  
160 2012, 2006). AIRS radiances at wavelengths from 8 to 12 μm are used here, excluding  
161 the 9.6 μm ozone band. The parent molecule H<sub>2</sub>O is retrieved at both 8 and 12 μm, but  
162 HDO is retrieved primarily from strong absorption lines in the 8 μm region (particularly  
163 in the wavenumber range 1210 to 1270 cm<sup>-1</sup>). Cloud optical depth and cloud top pressure  
164 are jointly retrieved with the chemical species, using the approach described in Kulawik  
165 et al. (2006). The cloud-clearing approach (Susskind et al., 2003), utilized in AIRS  
166 operational products up to and including AIRS v6, where retrievals are reported on the 45  
167 km AMSU footprint, is not utilized here. As described by Worden et al. (2019), retrievals  
168 are performed on single AIRS 13.5-km footprints in order to preserve the Level 1B  
169 radiance noise characteristics (Irion et al., 2018; DeSouza et al., 2018).

170

171 For H<sub>2</sub>O, the a priori constraint vectors come from NASA's Goddard Earth Observing  
172 System (GEOS) data assimilation system GEOS version 5.12.4 processing stream  
173 (Rienecker et al., 2008). These are produced by the Global Modeling and Assimilation  
174 Office (GMAO) at the NASA Goddard Space Flight Center (GSFC). The GMAO GEOS-  
175 5.12.4 water mixing ratios are linearly interpolated to the latitudes, longitudes, and



176 log(pressure) levels of satellite retrievals to generate the a priori profiles.

177

178 For all HDO retrievals, the initial profile of the HDO/H<sub>2</sub><sup>16</sup>O isotopic ratio is set equal to a  
179 simulated tropical profile (Worden et al., 2006). In the AIRS HDO product files, a priori  
180 HDO is defined as the product of the local a priori H<sub>2</sub>O profile (GMAO GEOS-5.12.4)  
181 and one tropical a priori profile of the HDO/H<sub>2</sub>O isotopic ratio (Worden et al., 2006). The  
182 initial guess profiles for H<sub>2</sub>O are set equal to the a priori.

183

### 184 **3.2 Method of comparison**

185 The AIRS HDO/H<sub>2</sub>O retrievals are matched up in space and time with the aircraft in situ  
186 HDO/H<sub>2</sub>O measurements. A critical aspect of validating satellite retrievals is obtaining  
187 data that span the altitudes where the satellite has sensitivity to HDO/H<sub>2</sub>O. AIRS data are  
188 sensitive to the HDO/H<sub>2</sub>O ratio in the atmosphere from the surface up to approximately  
189 10,000 m altitude. The aircraft samples HDO and H<sub>2</sub>O from the surface up to 6000 m  
190 altitude, spanning most of the altitudes where the AIRS data are sensitive and therefore  
191 allowing us to validate AIRS HDO/H<sub>2</sub>O with in situ measurements.

192

193 For direct comparison of AIRS HDO/H<sub>2</sub>O with in situ HDO/H<sub>2</sub>O, the AIRS instrument  
194 operator (averaging kernel and *a priori* constraint) is applied to the in situ data (see Eq. 1  
195 below), as described by Rodgers (2000). This has the effect of smoothing the in situ data  
196 to the same resolution as the satellite retrievals. The averaging kernel matrix  $A$  is the  
197 sensitivity of the AIRS estimate to the true concentration in the atmosphere (Rodgers,  
198 2000). The in situ profile with applied averaging kernel  $x_{in situ w/AK}$  is calculated jointly for



199 HDO and H<sub>2</sub>O using the AIRS operator:

$$200 \quad x_{insituw/AK} = x_a + A_{xx}(x - x_a) \quad (1)$$

201

202 Joint HDO/H<sub>2</sub>O retrievals are performed on the logarithm of the volume mixing ratios,  $x_D$   
203  $= \ln(q_D)$  and  $x_H = \ln(q_H)$  (Worden et al., 2012, 2006). The data structure for AIRS HDO  
204 files is similar to TES HDO, with details provided by Herman et al. (2014).

205

206 For comparison with AIRS, the in situ HDO and H<sub>2</sub>O profiles are extended to cover the  
207 full range of AIRS levels. In the boundary layer, from the surface up to the lowest  
208 altitude aircraft data, we assume constant values of HDO and H<sub>2</sub>O set equal to the first  
209 aircraft measurement. In the range of aircraft data (up to 6000-m flight ceiling), the  
210 aircraft in situ HDO and H<sub>2</sub>O data are interpolated to the levels of the AIRS forward  
211 model, smoothing fine scale features. In the layers above the aircraft maximum altitude,  
212 the profile is extrapolated using a scaled a priori profile. In this paper, all comparisons  
213 have been completed applying Eq. 1.

214

#### 215 **4 Validation**

216 Validating the accuracy of AIRS HDO and H<sub>2</sub>O retrievals is important for studies of the  
217 hydrologic cycle, exchange processes in the troposphere, and climate change.

218 Comparisons of AIRS and TES over five years (2006-2010) indicate that the retrieval  
219 characteristics of the AIRS HDO/H<sub>2</sub>O measurements have similar vertical resolution and  
220 uncertainty in the middle troposphere but with slightly less sensitivity in the lower  
221 troposphere (Worden et al., 2019). Worden et al. (2019) reported that the calculated



222 uncertainty of AIRS HDO/H<sub>2</sub>O is ~30 per mil for a tropospheric average between 750  
223 and 350 hPa, with mean bias between TES and AIRS (TES-AIRS) for the HDO/H<sub>2</sub>O  
224 ratio of ~-2.6 per mil and a latitudinal variation of ~7.6 per mil.

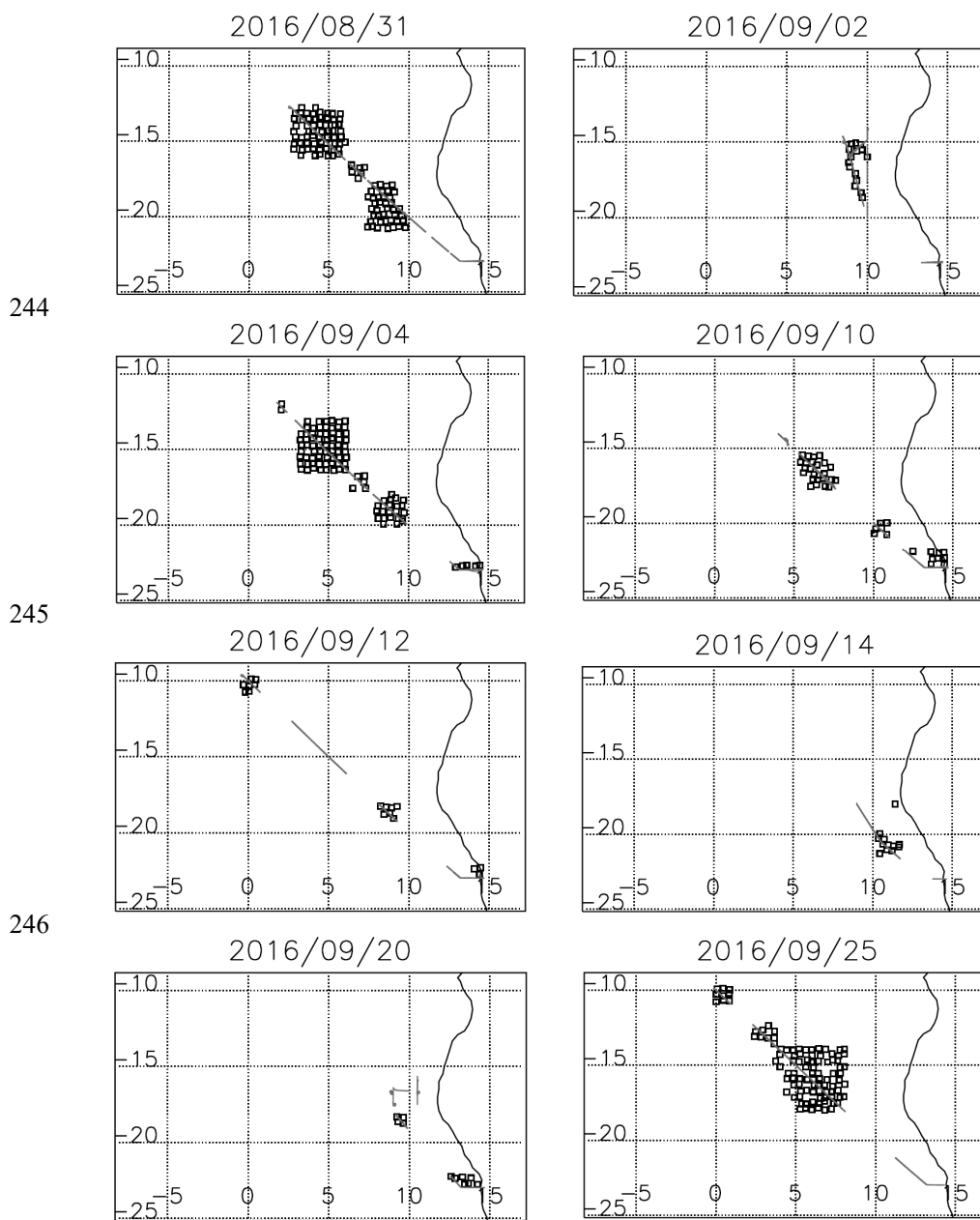
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#### 226 **4.1 Comparison of AIRS with Aircraft Measurements**

##### 227 **ORACLES 8/31 to 9/25/2016 data comparison.**

228 In this section, we describe comparisons between AIRS and ORACLES aircraft HDO  
229 measurements. First, time segments of each aircraft flight are identified where the aircraft  
230 profiled from the boundary layer up to approximately 6000 m altitude. To minimize the  
231 impact of atmospheric spatial and temporal variability, same-day AIRS measurements are  
232 selected for the same latitude/longitude rectangle as each aircraft profile (Fig. 2). These  
233 matched pairs are compared by the method described in Sect. 3.2. Within each flight are  
234 several profiles each spanning 1 to 3 degrees (or ~ 100 to 300 km), so measurement pairs  
235 are typically within 3 degrees (Fig. 2). The standard data retrieval quality flags for the  
236 retrieval are used in this analysis, which are based on the Aura TES data retrieval quality  
237 flags (Herman and Kulawik, 2018). For closer spatial coincidence, we also selected  
238 AIRS-aircraft measurement pairs within 0.3 degrees (Fig. 3). Following Worden et al.  
239 (2007) and Brown et al. (2008), we filter data for a reasonable threshold of DOFS (DOFS  
240 > 1.1), but include all cloud optical depths. Fig. 4(a) shows a representative 31 Aug 2016  
241 comparison between aircraft water vapor  $\delta D$  from WISPER and the coincident AIRS  
242 retrieval. Fig. 4(b) shows the corresponding averaging kernels.

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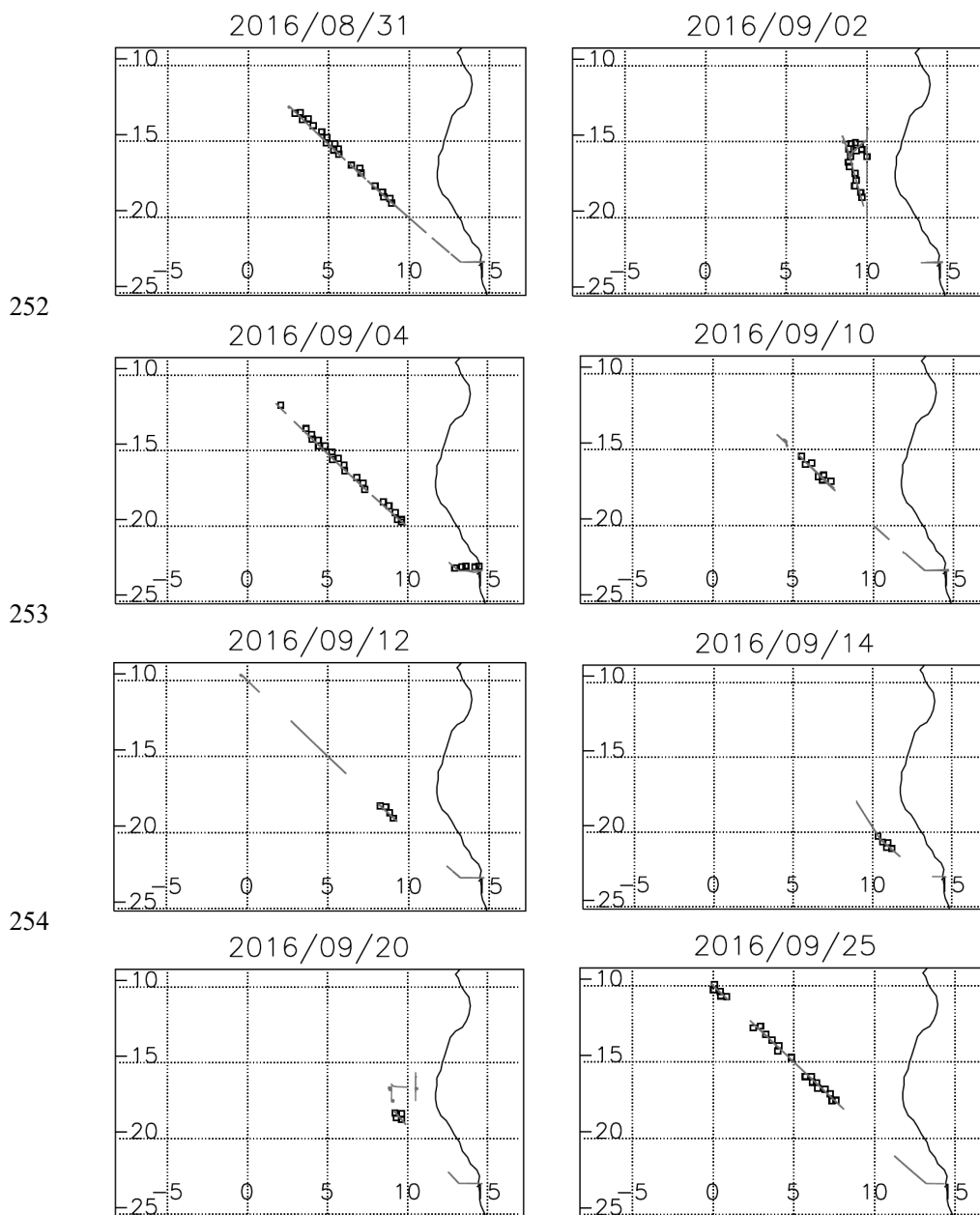
**Figure 2.** ORACLES aircraft profiles (thin grey line segments) over the southeast

249 Atlantic Ocean to the west of Africa are matched to AIRS fields of view (FOVs) (square

250 symbols) within the same latitude/longitude rectangle as the aircraft profiles for eight



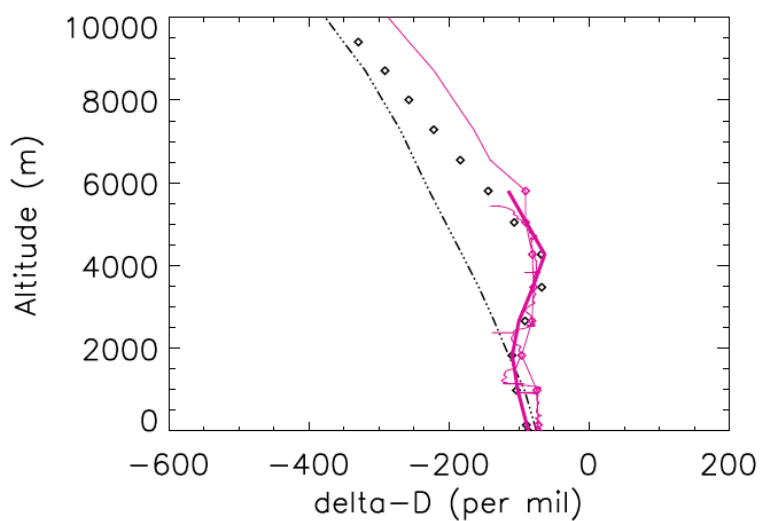
251 flights in 2016.



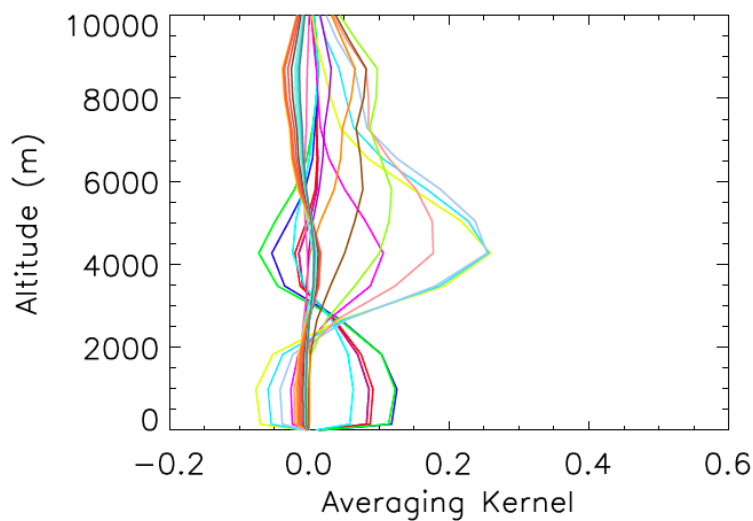
255  
256 **Figure 3.** In close spatial coincidence, ORACLES aircraft profiles (thin grey line  
257 segments) are matched within 0.3 degrees to AIRS FOVs (square symbols).



258



259



260

261 **Figure 4.** (a) Sample comparison of the  $\delta D$  profiles by aircraft and satellite over the  
262 southeast Atlantic Ocean during ORACLES on 31 August 2016: shown are AIRS  $\delta D$   
263 (black diamond symbols), the prior  $\delta D$  (black dash-dot-dot line), nearest WISPER  $\delta D$   
264 (thin red line), WISPER  $\delta D$  interpolated to satellite levels (red diamonds), and the  
265 WISPER  $\delta D$  with the AIRS averaging kernel applied (thick red line).



266 (b) Averaging Kernel corresponding to same AIRS profile on 31 August 2016, color-  
267 coded by pressure level. Averaging kernels with the largest positive sensitivity below  
268 2000 m are from the lowest altitudes.

269

#### 270 **4.2 AIRS Bias correction**

271 TES HDO/H<sub>2</sub>O ratios are biased compared to model and in situ measurements (Worden  
272 et al., 2006, 2007, 2011). We assess whether AIRS HDO has a bias relative to in situ  
273 measurements. As described above, AIRS and TES show a small bias for the HDO/H<sub>2</sub>O  
274 ratio of ~-2.3 per mil (Worden et al., 2019) after a bias correction is applied, so it is  
275 reasonable to see how well in situ and AIRS data agree if the TES bias correction is  
276 applied to the AIRS HDO. Herman et al. (2014) estimated the TES bias  $\delta_{bias}$  by  
277 minimizing the difference between bias-corrected TES and in situ  $\delta D$  with TES operator  
278 applied:

$$279 \quad \delta_{bias} = 0.00019 \times Pressure - 0.067 \quad (2)$$

280 We apply the TES  $\delta_{bias}$  to the AIRS data to evaluate against ORACLES aircraft data.  
281 There are 446 matched profiles of AIRS and ORACLES within the same  
282 latitude/longitude boxes (Fig. 2), and 110 closely-matched profiles within 0.3 degrees or  
283 approximately 30 km (Fig. 3). Comparisons with averaging kernel applied are shown in  
284 Fig. 5 and Table 2. Over the range of aircraft data, 0 km to 6 km altitude, AIRS  $\delta D$  has a  
285 mean bias of -6.7‰ relative to the aircraft profiles, well within the estimated  
286 measurement uncertainty of both AIRS and the WISPER calibration. This is consistent  
287 with TES  $\delta D$  (Worden et al., 2019; Herman et al., 2014). AIRS lower-tropospheric  $\delta D$   
288 bias is -6.6‰ and RMS 20.9‰ (surface to 800 hPa). In the mid-troposphere, 800 to 500

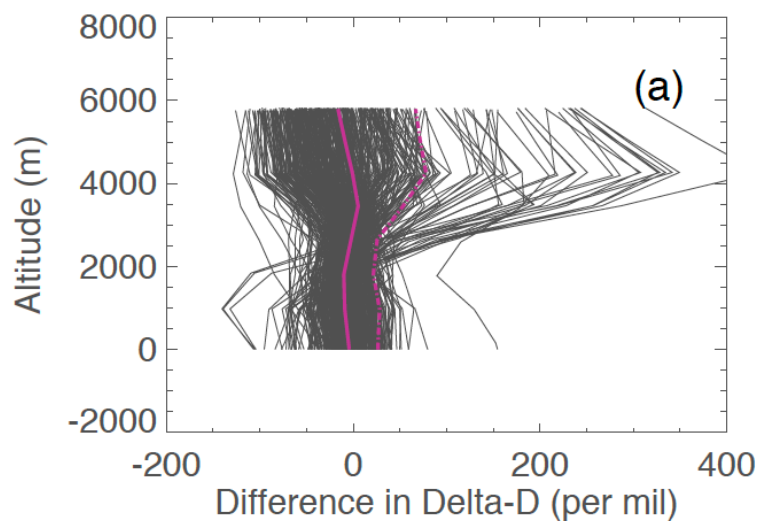




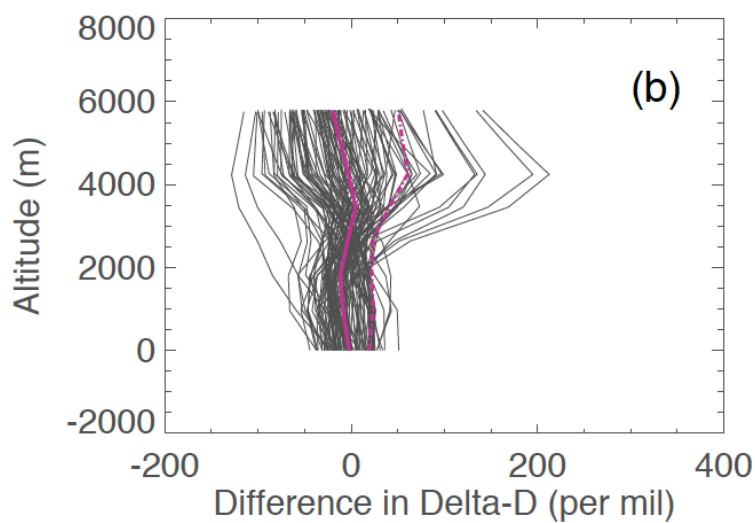
289 hPa, AIRS  $\delta D$  bias is -6.8% and RMS 44.9%.

290

292



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293

294 **Figure 5.** (a) AIRS minus ORACLES aircraft  $\delta D$  for the 446 matches within 3 degrees

295 (Fig. 2). Lines are individual profiles (black lines), mean (red solid line) and RMS (red



296 dash dot line).

297 **(b)** AIRS minus ORACLES aircraft  $\delta D$  for the 110 matches within 0.3 degrees (Fig. 3).

298

299 **Table 2.** Summary of satellite-aircraft comparisons for 110 matched pairs in 2016 (Fig. 3). Bias and RMS

300 (standard deviation) of AIRS  $\delta D$  relative to ORACLE aircraft with averaging kernel applied (“BiasAK”,

301 “RMSak”), and for AIRS relative to mapped ORACLES aircraft, no averaging kernel (“Bias”, “RMS”).

Altitude (m)	Pressure (hPa)	BiasAK (‰)	RMSak (‰)	Bias (‰)	RMS (‰)
0.01	1014.63	-2.46	18.98	-14.82	22.64
136.61	1000.00	-3.35	19.38	-18.14	22.79
968.87	908.51	-8.86	23.39	-0.31	131.50
1807.71	825.40	-11.80	22.05	9.77	89.68
2641.34	749.89	-3.89	22.63	-13.24	38.07
3456.36	681.29	4.89	41.03	-3.66	35.98
4250.29	618.97	-2.96	60.63	12.52	76.03
5027.62	562.34	-11.87	55.15	-16.62	73.75
5792.12	510.90	-20.09	50.61	-40.41	81.22

302

303

## 304 **5. Error estimation**

305 In this section we characterize the error budget for AIRS and assess this error by

306 comparison with the ORACLES aircraft measurements. Error analysis in optimal

307 estimation has been described in detail in the literature (Worden et al., 2004, 2006;

308 Bowman et al., 2004; Rodgers, 2000). The error  $\tilde{x}$  in the estimate of HDO/H<sub>2</sub>O is defined

309 as the true state  $x$  minus the linear estimate  $\hat{x}$  retrieved by AIRS (e.g., Worden et al.,

310 2006, Eq. (15)):



311 
$$\tilde{\mathbf{x}} = \mathbf{x} - \hat{\mathbf{x}}. \quad (3)$$

312 Similar to Herman et al. (2014), we define the *estimated error* of the AIRS isotopic ratio  
313 HDO/H<sub>2</sub>O, (Eq. 4) as the observation error covariance (Worden et al., 2006):

314 
$$\mathbf{S} = \mathbf{G}_R \mathbf{S}_n \mathbf{G}_R^T + \mathbf{G}_R \left( \sum_i \mathbf{K}_i \mathbf{S}_b^i \mathbf{K}_i^T \right) \mathbf{G}_R^T, \quad (4)$$

315 where  $\mathbf{G}_R = (\mathbf{G}_z^D - \mathbf{G}_z^H)$ ,  $\mathbf{S}_n$  is the measurement error covariance, and  $\mathbf{S}_b^i$  is the error  
316 covariance due to systematic errors and interference errors. The estimated error is given  
317 by the square roots of the diagonal elements of  $\mathbf{S}$ , the best estimate of the AIRS  
318 observation error covariance for the HDO/H<sub>2</sub>O retrieval. In the case where AIRS is  
319 compared to in situ measurements without the averaging kernel, there is an additional  
320 smoothing error.

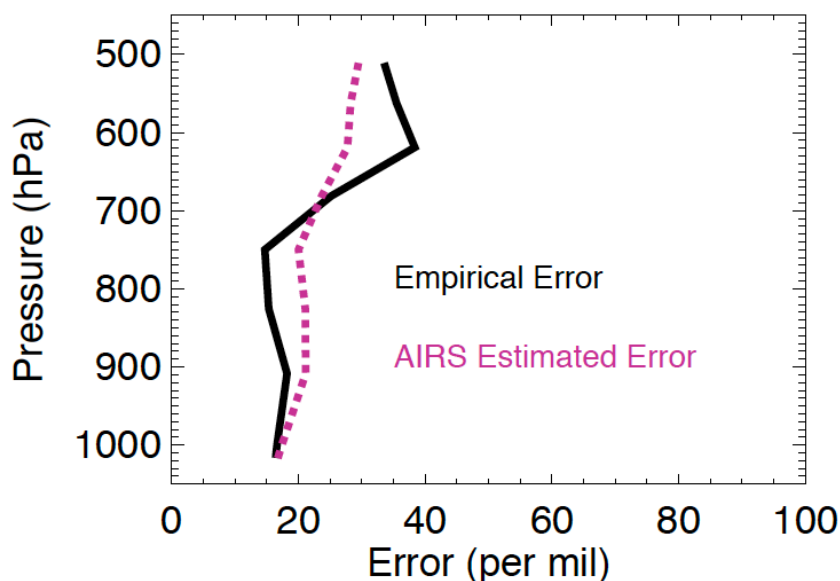
321

322 The estimated error (Eq. 4) is compared to the empirical error calculated from the AIRS-  
323 aircraft comparisons. It is seen that the error varies from ~20 to ~40 per mil (Fig. 6). The  
324 empirical error (AIRS versus aircraft RMS) is similar in magnitude to the estimated error,  
325 but exceeds the estimated error at 500 to 600 hPa in the free troposphere. These  
326 differences are likely due to atmospheric variability as we do not have exact matchups  
327 between the AIRS data and aircraft measurements.

328



329



330

331 **Figure 6.** AIRS error analysis for coincident AIRS and ORACLES  $\delta D$  on 31 August  
332 2016 shows the empirical error is comparable to the AIRS estimated error. Plotted are the  
333 AIRS  $\delta D$  estimated error also known as AIRS observation error (red dashed line) and the  
334 AIRS  $\delta D$  empirical error (black line).

335

336

## 337 **6. Conclusions**

338 HDO/H<sub>2</sub>O estimates from AIRS single footprint radiances been compared to coincident  
339 in situ airborne measurements on the P-3B Orion aircraft by the Oregon State Water  
340 WISPER system (Water Isotope Spectrometer for Precipitation and Entrainment  
341 Research) over the Southeast Atlantic Ocean. On eight days between 31 Aug and 25 Sep  
342 2016, there are collocated measurements between AIRS and the P-3B aircraft. We have



343 shown that AIRS-only retrievals have sensitivity to HDO from the middle troposphere to  
344 the boundary layer. We demonstrate that AIRS  $\delta D$  has a mean bias of  $-6.7\%$  relative to  
345 aircraft, well within the estimated measurement uncertainty. In the lower troposphere,  
346 1000 to 800 hPa, AIRS  $\delta D$  bias is  $-6.6\%$  and the RMS  $20.9\%$ , consistent with the  
347 calculated uncertainty of  $19.1\%$ . In the mid-troposphere, 800 to 500 hPa, AIRS  $\delta D$  bias  
348 is  $-6.8\%$  and RMS  $44.9\%$ , comparable to the calculated uncertainty of  $25.8\%$ .  
349



350 **Code/Data availability.** The ORACLES aircraft data used in the data analysis can be

351 freely downloaded from the following Digital Object Identifier:

352 ([http://dx.doi.org/10.5067/Suborbital/ORACLES/P3/2016\\_V1](http://dx.doi.org/10.5067/Suborbital/ORACLES/P3/2016_V1), last access: 22 April

353 2017). We expect the AIRS-based deuterium data to be publicly released by January

354 2020. Files in IDL format of the AIRS data shown and forward model output are

355 available from coauthor John Worden upon request: [john.r.worden@jpl.nasa.gov](mailto:john.r.worden@jpl.nasa.gov).

356

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358 Henze (DH), Kevin Bowman (KB), Karen Cady-Pereira (KC), Vivienne H. Payne (VP),

359 Susan S. Kulawik (SK), and Dejian Fu (DF).

360

361 **Author contribution.** RH carried out all steps of aircraft validation, from matching data

362 and quality filtering to applying observation operator and statistics, while JW provided

363 satellite-to-satellite validation. JW developed the retrieval strategies for both AIRS and

364 TES HDO/H<sub>2</sub>O retrievals. DF and SK built the strategies of single AIRS footprint

365 HDO/H<sub>2</sub>O retrievals into the MUSES algorithm. KC, RH and VP evaluated the

366 sensitivities of retrievals to the choice of forward model. RH, VP, JW, SK, DF, DN, DH

367 and KB contributed to the text and interpretation of the results. JW and SK helped in the

368 estimation of HDO/H<sub>2</sub>O measurement uncertainty, quality flagging and knowledge of the

369 retrieval process. DN and DH provided ORACLES data, aircraft measurement

370 uncertainty, and identified profiles in the aircraft data. All authors participated in writing

371 the manuscript.

372



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

374

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382



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