

**Title:** LEMON2021 Ground validation campaign

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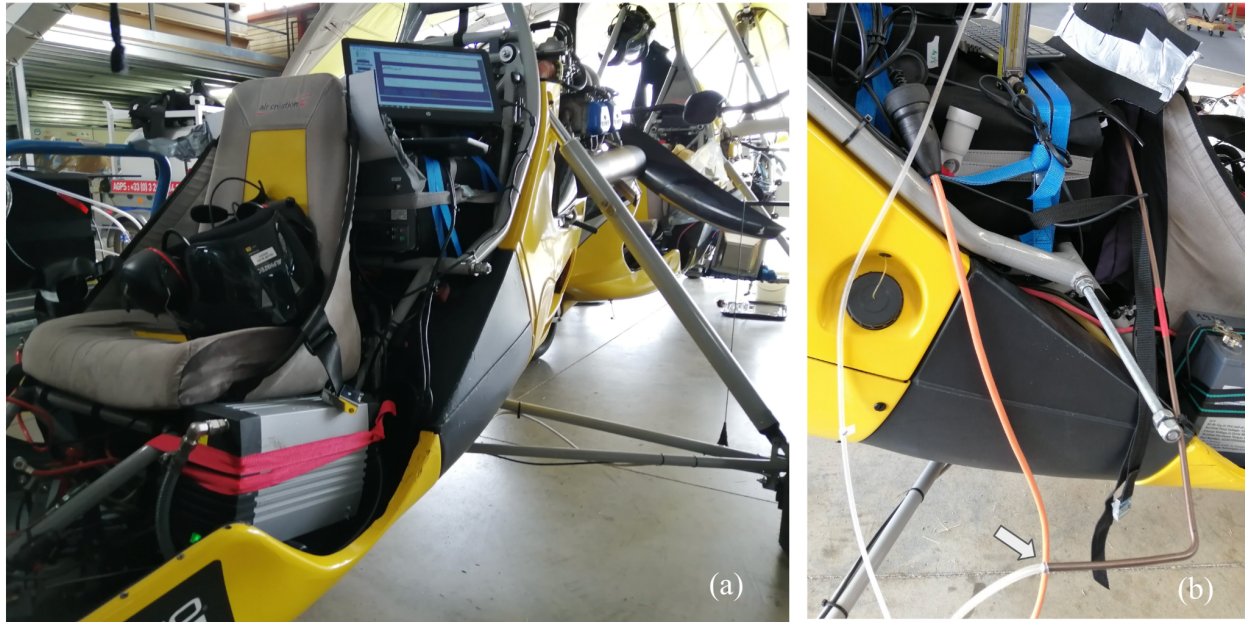
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## **Dataset description**

The LEMON CRDS ULA dataset consists of geolocated observations of humidity, water vapor isotopic composition, temperature and atmospheric pressure acquired with an ultralight aircraft (ULA) over the area of Aubenas (France) between 17/09/2021 and 23/09/2021. Data is provided in NetCDF format with 3 different averaging times for each flight (2, 5, 10 seconds). Take off location is an airstrip next to the Lanås Airfield (44.5393° N, 4.3679° E, 281 m ASL). The present document contains:

- Information about the setup of the water vapor analyzer in the ULA.
- Table 1, which reports the time (UTC), duration and maximum altitude for each flight.
- Table 2, in which are listed all the variables included in each NetCDF file and their units. For each variable, a short description with topical information is also reported.
- An explanation of the different isotope-humidity correction curves estimated with laboratory experiment and estimated with on-site characterization tests. The impact of the two corrections is also reported (Table 3 and Figures 3-7)

## Instrument setup in the ultralight aircraft



**Figure 1:** Installation of the Picarro L2130-i in the ULA. **(a)** the analyzer wrapped in neoprene insulation material is placed on the back seat of the ULA. The vacuum pump is visible at the side of the pilot's seat. **(b)** Detail of the inlet. The white arrow highlights the tip of the inlet, covered during servicing in the hangar.

The ULA equipped with a water vapor isotope analyzer is visible in Figure 1. The analyzer was placed on the back seat of the ULA and wrapped with a neoprene sheet for thermal insulation. Ambient air was sampled by the CRDS analyzer in flight mode at a nominal flow rate of 80 sccm through an unheated inlet of 80 cm length made of stainless steel (Silconert coating). The inlet was pointing backward on the right side of the aircraft. During servicing, the inlet was covered with a  $0.45\ \mu\text{m}$  polyethersulfone filter to prevent the analyzer sampling dirt, dust particles and exhaust gasses. The filter was removed before take off.

**Table 1:** Flight details. Start and stop time in UTC.

\* GPS data not available. Altitude can be estimated by readings of ambient pressure.

\*\*Injection of standard water vapor between 17:27:30 to 17:47:42.

Flight name	Date (YYYY-MM-DD)	Start (HH:MM:SS)	Stop (HH:MM:SS)	Duration (HH:MM:SS)	Max. Altitude (m ASL)
LEMON2021_f02	2021-09-17	13:31:00	14:26:00	00:55:00	NA*
LEMON2021_f03	2021-09-17	15:21:00	16:48:00	01:27:00	NA*
LEMON2021_f04	2021-09-18	05:12:00	05:12:00	01:00:00	1669
LEMON2021_f05	2021-09-18	08:12:00	09:32:00	01:20:00	1730
LEMON2021_f06	2021-09-18	12:15:00	13:10:00	00:55:00	1751
LEMON2021_f07	2021-09-18	14:54:00	16:13:00	01:19:00	3157
LEMON2021_f08	2021-09-19	07:56:00	09:30:00	01:34:00	2166
LEMON2021_f09	2021-09-20	06:42:00	08:28:00	01:46:00	2161
LEMON2021_f10	2021-09-20	09:37:00	10:53:00	01:16:00	1254
LEMON2021_f11	2021-09-20	16:04:00	17:46:00	01:42:00	3120
LEMON2021_f12	2021-09-21	06:56:00	08:38:00	01:42:00	3173
LEMON2021_f13**	2021-09-21	17:08:00	19:00:00	01:52:00	1579
LEMON2021_f14	2021-09-22	08:00:00	09:55:00	01:55:00	3141
LEMON2021_f15	2021-09-22	13:00:00	15:07:00	02:07:00	3204
LEMON2021_f16	2021-09-23	08:04:00	09:47:00	01:43:00	3163

**Special notes:**

- For flight f02 and f03 the GPS sensor was not working properly. Altitude can be estimated by the pressure readings (p) installed inside the L2130-i.
- Flight f02 was performed after suboptimal instrumental warm-up.
- The L2130i instrument was rebooted on 23-09-2022. Last instrumental calibration performed just before f16.

**Table 2:** Variable description.

\*Measured on the field.

Name	Unit	Instrument/Sensor	Description
ALT	m	GPS onboard iMet XQ2	Altitude in meters above sea level
d	‰ (VSMOW-SLAP)	Picarro L2130-i	Water vapor d-excess calculated from delta_18O and delta_D (using laboratory humidity correction)
delta_18O	‰ (VSMOW-SLAP)	Picarro L2130-i	Water vapor $\delta^{18}\text{O}$ with laboratory humidity correction Precision ( $1\sigma$ , 10 sec, 2500 ppmv): 0.25‰ Precision ( $1\sigma$ , 10 sec, 12500 ppmv): 0.12‰ Response Time (63.2%): 5.75 s* Response Time (99.3%): 28.75 s*
delta_18O_FC	‰ (VSMOW-SLAP)	Picarro L2130-i	Water vapor $\delta^{18}\text{O}$ with humidity correction curve estimated in the field
delta_18O_FC_OF	‰ (VSMOW-SLAP)	Picarro L2130-i	Similar to delta_18O_FC but implementing an optimal filter to account for the impulse response of the system
delta_18O_OF	‰ (VSMOW-SLAP)	Picarro L2130-i	Similar to delta_18O but implementing an optimal filter to account for the impulse response of the system
delta_D	‰ (VSMOW-SLAP)	Picarro L2130-i	Water vapor $\delta\text{D}$ with laboratory humidity correction Precision ( $1\sigma$ , 10 sec, 2500 ppmv): 1.6‰ Precision ( $1\sigma$ , 10 sec, 12500 ppmv): 0.3‰ Response Time (63.2%): 6.72 s* Response Time (99.3%): 33.58 s*
delta_D_FC	‰ (VSMOW-SLAP)	Picarro L2130-i	Water vapor $\delta\text{D}$ with humidity correction curve estimated in the field
delta_D_FC_OF	‰ (VSMOW-SLAP)	Picarro L2130-i	Similar to delta_D_FC but implementing an optimal filter to account for the impulse response of the system
delta_D_OF	‰ (VSMOW-SLAP)	Picarro L2130-i	Similar to delta_D but implementing an optimal filter to account for the impulse response of the system
event	-	Post-processing	Event identifier for FARLAB-UiB calibration
flag	-	Post-processing	Quality flag after FARLAB-UiB calibration
H2O_FC	ppmv	Picarro L2130-i	Water vapor volume mixing ratio calibrated on the field Response Time (63.2%): 5.19 s* Response Time (99.3%): 25.93 s*
H2O_FC_OF	ppmv	Picarro L2130-i	Similar to H2O_FC but implementing an optimal filter to account for the impulse response of the system
H2O_OF	g kg <sup>-1</sup>	Picarro L2130-i	Similar to q but implementing an optimal filter to account for the impulse response of the system
LAT	decimal degrees north	GPS onboard iMet XQ2	Latitude
LON	decimal degrees east	GPS onboard iMet XQ2	Longitude
outvalve	-	Picarro L2130-i	Picarro L2130-i outlet proportional valve [0-65535]

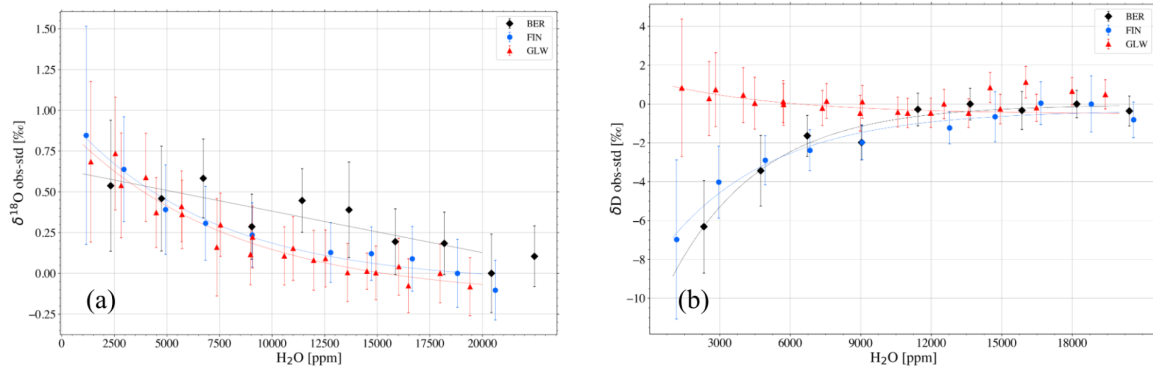
P	hPa	Pressure transducer onboard iMet XQ2	Atmospheric pressure measured on ULA mast. Response Time: 10 ms Accuracy: +/- 1.5 hPa Resolution: 0.01 hPa
p	hPa	Picarro L2130-i	Atmospheric pressure measure by transducer mounted inside the Picarro L2130-i enclosure
pc	torr	Picarro L2130-i	Cavity pressure
q	g kg <sup>-1</sup>	Picarro L2130-i	Calculated from Picarro L2130-i volume mixing ratio
SATCNT	-	GPS onboard iMet XQ2	Number of satellites for GPS position
TA	°C	Bead thermistor onboard iMet XQ2	Air temperature Response Time: 1 second @ 5m/s flow Accuracy: +/- 0.3° C Resolution: 0.01° C
Tc	°C	Picarro L2130-i	Cavity temperature
TD	°C	Calculated by iMet XQ2	Dew Point temperature
Tdas	°C	Picarro L2130-i	Data Acquisition System temperature
time	days	GPS onboard iMet XQ2	GPS time (UTC). Time elapsed since 00:00:00 1-Jan-1970 UTC
Twb	°C	Picarro L2130-i	Warm Box temperature
UU	%	Capacitive humidity sensor onboard iMet XQ2	Relative humidity in percent Response Time: @ 25C, 0.6s; @ 5C, 5.2s; @ -10C, 10.9s Accuracy: +/- 5% RH Resolution: 0.1% RH
vmask	-	Picarro L2130-i	Picarro L2130-i valve mask status [0-64]

## Differences between water vapor $\delta^{18}\text{O}$ and $\delta\text{D}$ corrected with humidity-isotope characterization curves estimated in the lab and in the field

Raw measurements of water vapor isotopic composition were corrected for the mixing ratio-isotopic composition dependency of the instrument (HIDS2254) in two different ways before applying a 2-points calibration using water isotope standards. In general, the two methods consist in a systematic investigation of the mixing ratio dependency by injecting water vapor of known and constant isotopic composition at different humidity levels. The main difference between the two methods is the mathematical approach to correct the raw observations and when/where the tests were performed:

1. in the laboratory before the field campaign, using an extended number of experiments following Weng et al. (2020).
2. on-site during the field campaign, with 4 dedicated experiments using 3 different water vapor standards.

While the first correction is thoroughly discussed in Weng et al. (2020), the reader can find a brief description of the second correction hereafter. Figure 2 reports the mixing ratio-isotope composition dependency curves estimated in the field using three different standards: average BER (n. tests = 1), FIN (n. tests = 1), average GLW (n. tests = 2). The dependency is reported as a difference between observed delta values and the value of the same standard at a target mixing ratio.



**Figure 2:** Mixing ratio-isotope composition dependency of the Picarro HIDS2254 instrument as measured in the field. **(a)**  $\delta^{18}\text{O}$ , target humidity is 20434 ppm for BER, 18813 ppm for FIN and 17994 for GLW. **(b)**  $\delta\text{D}$ , target humidity is 18191 ppm for BER, 18813 ppm for FIN and 12543 ppm for GLW. Exponential best fits models are used to approximate the mixing ratio-isotope composition (lines).

The correction is a two-step process. First, the relative deviation of raw observation from the two standards that brackets the observation is calculated as follows:

$$x = \frac{\delta_{raw} - \delta_{FIN}}{\delta_{GLW} - \delta_{FIN}}$$

Where  $\delta_{raw}$  is the raw observation and  $\delta_{FIN}$  and  $\delta_{GLW}$  are the true values of the standards. Afterwards, the modeled value of each standards are calculated as follows:

$$\delta_{BASE} = \left( \beta_{0-FIN} + \beta_{1-FIN} * e^{(\beta_{2-FIN} * H_2O_{target-FIN})} \right) * (1 - x) + \left( \beta_{0-GLW} + \beta_{1-GLW} * e^{(\beta_{2-GLW} * H_2O_{target-GLW})} \right) * x$$

$$\delta_{OBS} = \left( \beta_{0-FIN} + \beta_{1-FIN} * e^{(\beta_{2-FIN} * H_2O_{meas})} \right) * (1 - x) + \left( \beta_{0-GLW} + \beta_{1-GLW} * e^{(\beta_{2-GLW} * H_2O_{meas})} \right) * x$$

Where  $\square_0$ ,  $\square_1$ ,  $\square_2$ , are the parameters of the best fit model estimated with least squares for FIN and GLW standards,  $H_2O_{target}$  is the reference level at which the corrected delta values will be reported and  $H_2O_{meas}$  is the observed humidity associated to the raw isotopic value. Finally, the corrected delta value of water vapor is calculated as follows:

$$\delta_{corr} = \delta_{raw} - (\delta_{OBS} - \delta_{BASE})$$

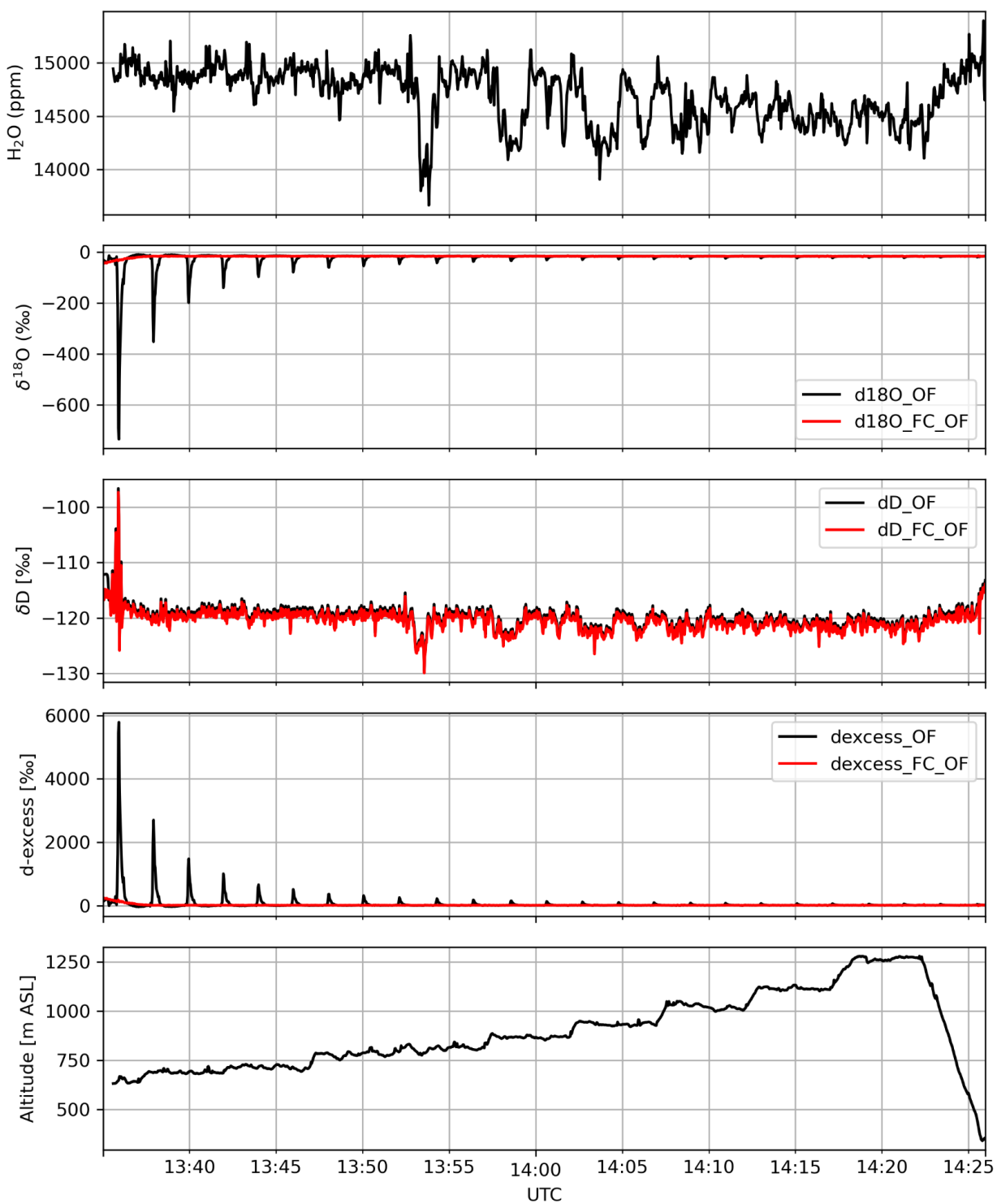
The corrected delta values are then calibrated in the field by using 15' to 30' long injections of 2 standards at a constant level, usually between 17000 and 18000 ppm.

In general, the difference between the two corrections is small and comparable to the instrumental precision, as shown in Table 3. In general, differences in isotopic composition are more pronounced for low humidity - high altitude flights. Figures 3 - 7 show the time series of water vapor isotopic compositions for flights with a pronounced difference in the final output between the two correction methods: f02, f07, f12, f15, f16.

**Table 3:** Mean absolute differences between final calibrated data corrected with laboratory and on-field mixing ratio-isotope composition dependency. All values in ‰. Underlined value when  $\delta^{18}O > 0.25\text{‰}$  |  $\delta D > 1\text{‰}$ .

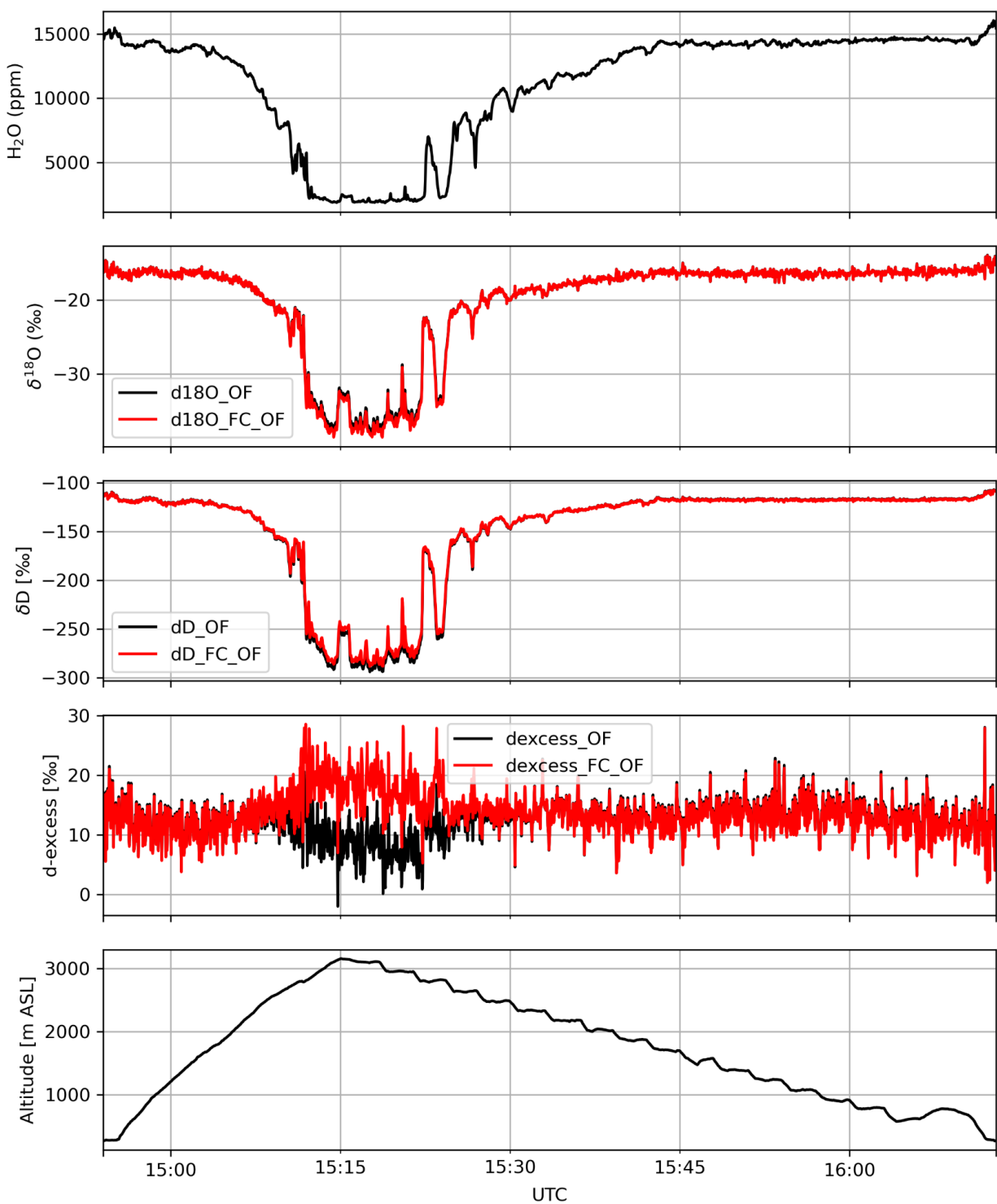
	f02*	f03	f04	f05	f06	f07	f08	f09	f10	f11	f12	f13	f14	f15	f16
$\delta^{18}O$	<u>0.25</u>	0.22	0.02	0.01	0.01	0.09	0.02	0.14	0.14	0.02	<u>0.30</u>	0.41	0.16	0.22	<u>0.50</u>
$\delta D$	0.55	0.47	0.26	0.25	0.32	<u>1.14</u>	0.55	0.29	0.14	0.69	<u>1.90</u>	0.82	0.97	<u>1.50</u>	<u>1.82</u>
d-excess	1.53	1.41	0.30	0.28	0.25	1.79	0.42	1.00	0.97	0.77	0.95	2.65	1.06	1.25	2.41

\*Calculated with data between 13:35:00 and 14:26:00 (UTC).

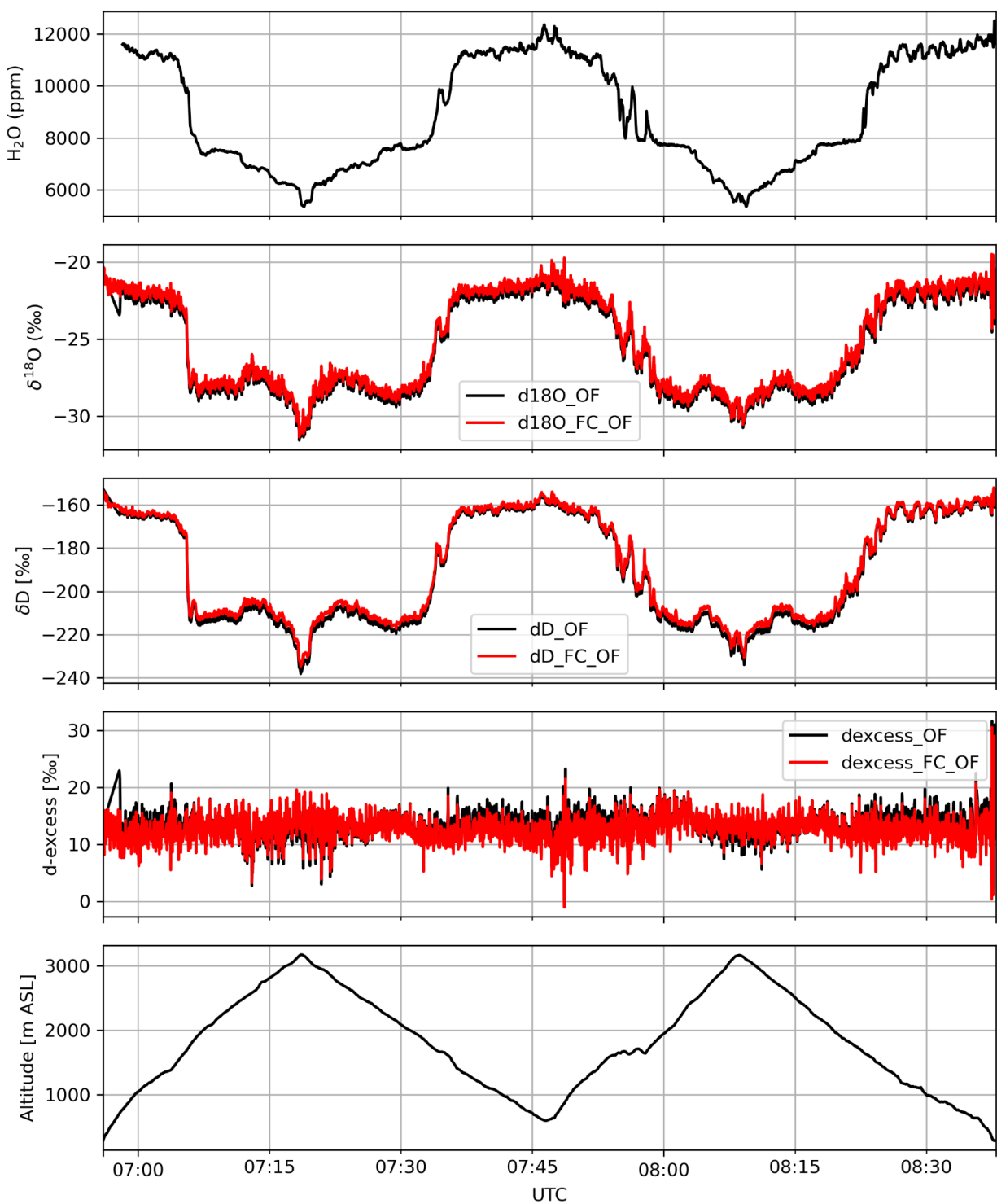


**Figure 3:** Difference between laboratory correction and field correction methods for f02. OF subscript means Optimal Filter.

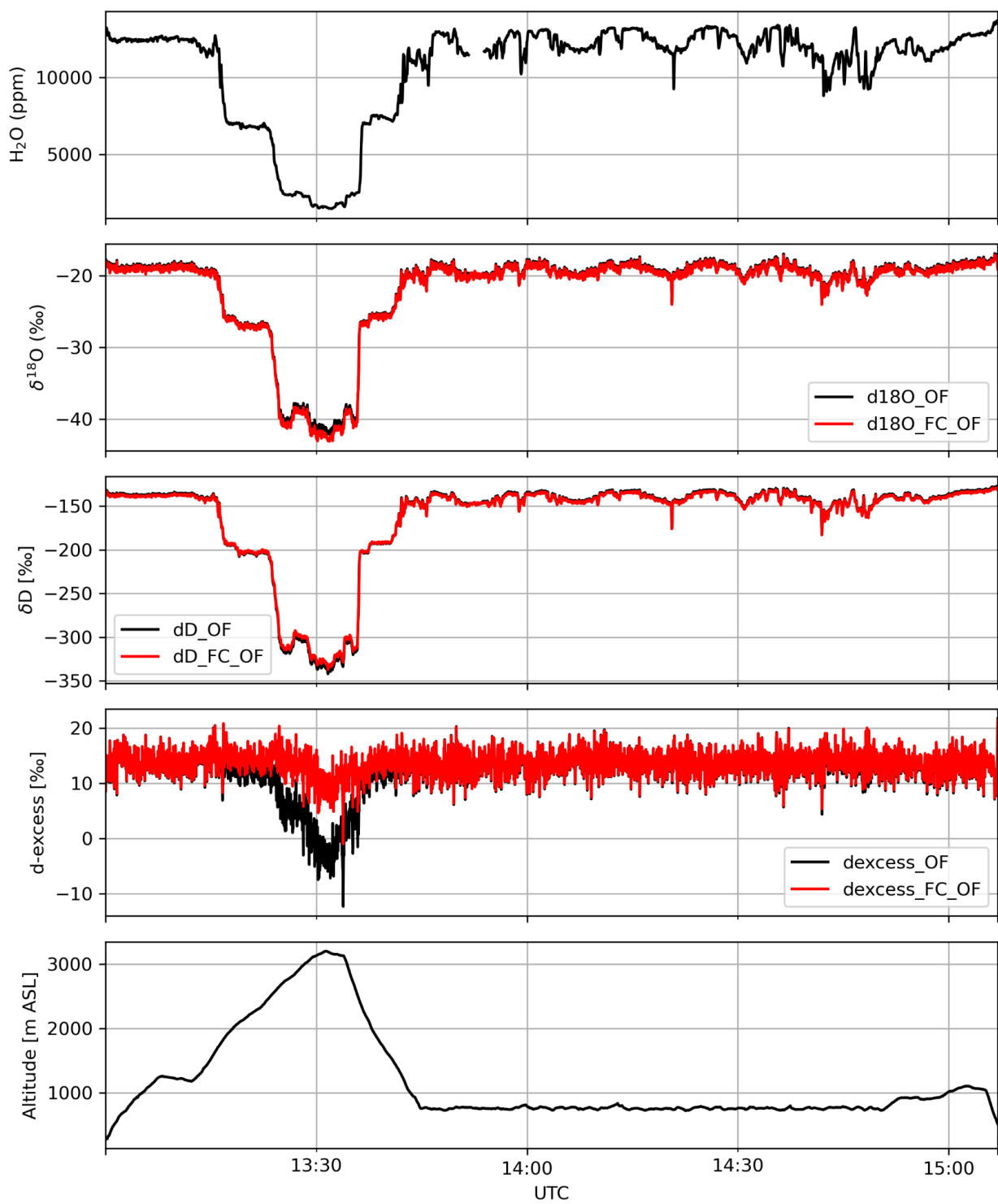




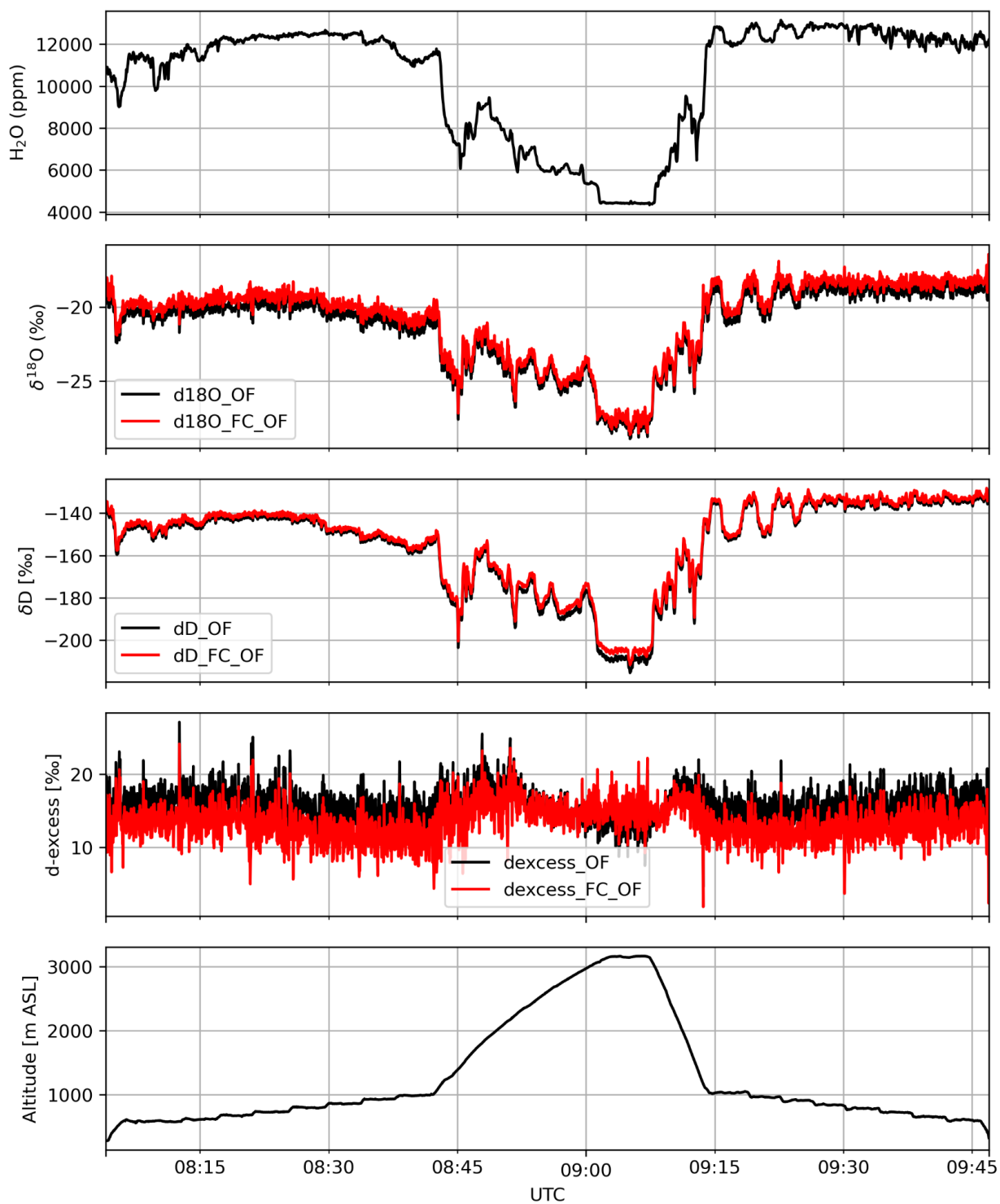
**Figure 4:** Same as for Figure 2 but for f07.



**Figure 5:** Same as for Figure 2 but for f12.



**Figure 6:** Same as for Figure 2 but for f15.



**Figure 7:** Same as for Figure 2 but for f16.

## References

Weng, Y., Touzeau, A., & Sodemann, H. (2020). Correcting the impact of the isotope composition on the mixing ratio dependency of water vapour isotope measurements with cavity ring-down spectrometers. *Atmospheric Measurement Techniques*, 13(6), 3167–3190. <https://doi.org/10.5194/amt-13-3167-2020>