Operational Instrument Description and Logfile for FARLAB water vapour isotope instrument HKDS2038

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This report documents the properties, calibration, events, and usage of instrument HKDS2038, owned by and operated according to principles set up by FARLAB at the Geophysical Institute (GFI) and the Department of Geosciences (GEO), University of Bergen (UiB), Norway. This particular instrument has been in use at FARLAB since 21.11.2016, in the laboratory for freshwater sample analysis, and in several occasions it has been deployed for water vapour measurements.

1 Instrument properties

The Picarro L2140-i with serial number HKDS2038 (Picarro Inc, Sunnyvale, USA) records at a data rate of ~ 1.25 Hz and with a air flow of ~ 35 sccm through the cavity. To minimize instrument drift and errors from the spectral fitting, these CRDS systems precisely control the pressure and temperature of

their cavities to be at $80 \pm 0.02^{\circ}$ C and 50 ± 0.1 Torr. The L2140-i for FARLAB has a so-called low humidity option, which means its cavity should be able to take measurements down to 200 ppmv, and a rack mount brackets for standard 19 inch racks.

For the spectral fitting, the instruments target three absorption lines of water vapour in the region 7199-7200 cm⁻¹ (Steig et al., 2014). In CRDS, a laser saturates the measurement cavity at one of the selected absorption wavelengths. After switching the laser off, a photodetector measures the decay (ring-down) of photons leaving the cavity through the semi-transparent mirrors (slightly less than 100% reflectivity). The ring-down time is inversely related to the total optical loss in the cavity. For an empty cavity, the ring-down time is determined solely by the reflectivity of the mirrors. For a cavity containing gas that absorbs light, the ring-down time will be shorter due to the additional absorption from the gas. The absorption intensity at a particular wavelength can be determined by comparing the ring-down time of an empty cavity to the ring-down time of a cavity that contains gas. The absorption peak is proportional to the concentration of molecule that generated the signal. The height or underlying area of each absorption peak is calculated based on the proper fitting of the absorption baseline. At lower water vapour concentrations, the signal-to-noise ratio decreases, and fitting algorithms are affected by various error sources (Weng et al., 2020).

The L2140-i in addition has a 17-O mode. Here, instead of cavity length, the laser current is modified to finely tune its frequency (Steig et al., 2017). At FARLAB, 17-O mode is so far only used for liquid injections.

2 Instrument calibration

This section summarises calibration experiments for the individual measurement parameters of the instrument.

2.1 Mixing ratio calibration

Water concentration measured by Picarro L2140-i was calibrated against dew point generator (LI-610, LI-COR Inc., Lincoln, NE, USA) on 2016-06-06 at FARLAB, UiB. The response to mixing ratio changes is rather linear over a wide range, with some uncertainty at low humidity, where the offset can lead to negative values during calibration (Fig. 2). The linear fits are y = 0.85231x - 719.55 for air as matrix gas, and y = 0.84183x - 639.45 for N₂ as matrix gas.

A final calibration will be performed with a dew point hygrometer.

2.2 Isotope composition – mixing ratio dependency

The Picarro L2140-i CRDS analysers have an optimal performance within a water vapour mixing ratio of 19000 – 21000 ppmv (parts per million by volume), where high signal-to-noise ratios enable precise measurements, such as for liquid sample analysis. In-situ measurements of the atmospheric water vapour isotopes vary widely, from 200 ppmv to more than 25000 ppmv. At low water vapour mixing ratios, the measurement uncertainty increases due to weaker absorption, and thus lower signal-to-noise ratios. Additionally, outside of this range, the measurement suffers from a mixing ratio-dependent deviation of the isotope composition. Since atmospheric mixing ratios can vary from below 500 ppmv in dry regions (e.g., polar regions or the middle and upper troposphere) to 30000 ppmv or more in humid regions (e.g., tropics), an appropriate correction to this mixing ratio dependency for high-quality in situ measurements of atmospheric water vapour is required (Weng et al., 2020).

So far there has not yet been done a systematic analysis for synthetic air as matrix gas, but for N_2 there is a systematic study by Weng et al., 2020 (Fig. 2; their Figure A2).



Figure 1: Calibration of mixing ratio from dewpoint generator experiments (FARLAB report 02-2017)



Figure 2: Isotope-composition mixing ratio dependency for instrument HKDS2038 determined with matrix gas N_2 using liquid injections (Weng et al., 2020, their Fig. A2).

3 Instrument events log

3.1 Fieldwork and locations

So far instrument was generally located at FARLAB, on several occasions at the GFI tower for water vapour measurements, and in 2018 the instrument was taken to a cruise on R/V Alliance, KV Svalbard, and Finse (Table 1).

3.2 Maintenance and repair

The instrument is used now exclusively for freshwater injections, avoiding issues as for the saltwater Picarro HKDS2039. Instrument degradation will have to be monitored through drift standards.

The instrument had a degradation in laser measurement frequency, which lead to lower data quality during the INTAROS cruise (Sep 2018). This may also have lead to instrument failure and degraded

temperature stability when installed at Finse (Dec 2018). Picarro suggested first resetting the heat element breakers, then replacing the hot box fans, which was done at FARLAB in 2018. The next modification was detaching and reattaching all laser cables in the Picarro, which may have become loose during one of the cruises. This helped to get the instrument back into operation.

During liquid injections, the instrument reacts to certain valve configurations with a reduced measurement frequency, which leads to bad injections. These are identified and removed when processing runs with the FLIIMP software. It may be possible to solve the problem by excluding certain valve states during vapourizer cleaning in the liquid injection ini file.

In some cases the 17-O mode would not be starting. Picarro support recommended restarting software with analyzer connected to ambient. This solution (shutting down N2 supply so that instrument draws ambient air from WLM tubing) helped the analyzer to stabilize after some time (30-120 min).

4 Data access, curation, use

Data is available with a Creative Commons license (attribution, access, re-use) after a 2-year carence period. Data are archived on the Bjerknes Centre Data Centre (BCDc, https://www.bcdc.no). The contact persons for data access are the data collectors stated above.

Further details on data storage, backup, processing and calibration is available in FARLAB report 2020-02 (https://wiki.uib.no/farlabprotocols/index.php/Main_Page).

5 References

- Weng, Y.: Instrument calibration of Picarro L2130-i (HIDS2254), FARLAB report 03-2017, 4 July 2017 (Version 2), 7 pp.
- Steig, E., Gkinis, V., Schauer, A., Schoenemann, S., Samek, K., Hoffnagle, J., Dennis, K., and Tan, S.: Calibrated high-precision 17O-excess measurements using cavity ring-down spectroscopy with laser-current-tuned cavity resonance, Meas. Tech, 7, 2421-2435, 2014.
- Weng, Y., Touzeau, A. and 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, Atmos. Meas. Techn., accepted.

6 Instrument usage

This section gives an overview over special event for the instrument, including relocations and field deployments. More specific events and an overview over data availability are given as standardised overview figures.

There are periods where the raw data are no longer available, but the injection files are (Jan–Nov 2016).

21.11.2016 to 15.02.2018	Instrument installed at FARLAB
25.02.2018 to 22.03.2018	Instrument installed on R/V Alliance for IGP campaign
30.07.2018 to 18.08.2018	Instrument installed onboard KV Svalbard for INTAROS
12.09.2018 to 02.12.2018	Instrument installed at FARLAB
02.12.2018 to 08.12.2018	Instrument installed at Finse for SNOWPACE
10.12.2018 to 06.01.2019	Maintenance at GFI
07.01.2019 to	Instrument installed at FARLAB
27.07.2019	Instrument moved to DI lab for microdrop testing
13.09.2019	Instrument returned to CF lab
11.03.2020 to 13.05.2020	Instrument installed at Finse for SNOWPACE

Table 1: Relocation and field deployment log

6.1 Events log for 2016

The standardised event log for 2016 is show in Fig. 3 $\,$

Table 2: Events log for 2016

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Figure 3: Data availability for the HKDS2038 during 2016 for (a) JFM (b) AMJ (c) JAS (d) OND.

6.2 Events log for 2017

The standardised event log for 2017 is show in Fig. 4

Table 3: Events log for 201	7	
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06.01.2017	Isotope composition – mixing ratio dependency
14.02.2017	Instrument shut down because of autosampler transfer
17.03.2017	Autosampler reinstalled and trained
06.06.2017 to $07.06.2017$	Measurements in O-17 mode
13.06.2017 to $14.06.2017$	Measurements in O-17 mode
28.07.2017 to 15.08.2017	Measurements in O-17 mode
20.10.2017	Instrument shut down
31.10.2017	Instrument restarted

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Figure 4: Data availability for the HKDS2038 during 2017 for (a) JFM (b) AMJ (c) JAS (d) OND.

6.3 Events log for 2018

The standardised event log for 2018 is show in Fig. 5

Table 4: Events log for 2018

13.02.2018	Isotope composition – mixing ratio dependency
16.02.2018	Instrument shutdown for shipping to Iceland
25.02.2018 to 22.03.2018	Instrument installed on R/V Alliance for IGP campaign
30.07.2018 to 18.08.2018	Instrument installed on KV Svalbard for INTAROS campaign
12.09.2018	Instrument installed at FARLAB with coated vapourizer $\#1$
17.09.2018	Modified scheme with different valve/pump sequence for cleaning
03.12.2018 to 08.12.2018	Instrument installed at Finse
10.12.2018 to $06.01.2019$	Maintenance work at GFI



Figure 5: Data availability for the HKDS2038 during 2018 for (a) JFM (b) AMJ (c) JAS (d) OND.

6.4 Events log for 2019

The standardised event log for 2019 is show in Fig. 6

Table 5: Events lo	g for 2019
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07.01.2019	Instrument reinstalled at FARLAB with salt vapourizer $#3$
09.05.2019 to 31.05.2019	Instrument run in 17-O mode
27.07.2019	Instrument moved to DI lab for microdrop testing
13.09.2019	Instrument returned to CF lab
25.12.2019 to 02.01.2020	Isotope-composition – mixing ratio dependency



Figure 6: Data availability for the HKDS2038 during 2019 for (a) JFM (b) AMJ (c) JAS (d) OND.

6.5 Events log for 2020

The standardised event log for 2020 is show in Fig. 7

Table 6: Events log for 2020

23.01.202	0 to 11.02.2020	Instrument in 17-O mode
10.03.202	0	Instrument shutdown for shipment
11.03.202	0 to 13.05.2020	Instrument installed at Finse for SNOWPACE
25.05.202	0	Instrument installed at FARLAB
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Figure 7: Data availability for the HKDS2038 during 2020 for (a) JFM (b) AMJ (c) JAS (d) OND.