Operational Instrument Description and Logfile for FARLAB water vapour isotope instrument HKDS2039

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This document documents the properties, calibration, events, and usage of instrument HKDS2039, 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 14.01.2016, mostly in the laboratory for saltwater and freshwater sample analysis, in a few occasions it has been deployed for water vapour measurements.

1 Instrument properties

The Picarro L2140-i with serial number HKDS2039 (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 03-2017)



Figure 2: Isotope-composition mixing ratio dependency for instrument HKDS2039 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 mostly 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 Kronprins Haakon (Table 1).

3.2 Maintenance and repair

No maintenance and repair issues so far. The instrument is used now for saltwater injections, which over time might cause requirement to change filters inside the Picarro. Using a salt liner below the septum and irregular vapourizer washing should remove salt from the evaporation system. Instrument degradation will have to be monitored through drift standards. Syringes suffer quite a lot of wear with the saltwater. A cleaning routine has been used that washes in DI. In addition, soaking the syringe in DI when not in use/after cleaning may be helpful.

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, while the injection files are (Jan–Nov 2016; Aug–Nov 2017).

2016-01-14 to 2018-03-15	Installation and operation at FARLAB
2018-03-16 to 2018-03-22	Installation at GFI tower
2018-03-22 to 2018-09-19	Installation at FARLAB
2018-09-27 to 2018-10-17	Installation on board R/V Kronprins Haakon (AeN)
2018-10-21 to 2018-12-03	Installation at FARLAB
2018-12-18 to 2019-02-08	Installation at GFI tower (SNOWPACE2018)
2019-02-08 to 2020-01-28	Installation at FARLAB
2020-01-28 to 2020-02-05	Installation at DI lab for Microdrop calibration tests
2020-02-11 to now	Installation at CF lab

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

2016	-01-14 to 2016-04-30	Memory experiments
2016	-06-03 to 2016-06-08	Absolute humidity calibration
2016	-06-22	WICO2016 IAEA stable water isotope intercomparison
2016	-06-28	"Marathon" (drift) test with 150 injections
2016	-12-08	Modified CoordinatorLIMS_G2000_A0325.ini file for mixing ratio dependency tests
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Figure 3: Data availability for the HKDS2039 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	g for	2017
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2017-01-06	Modified CoordinatorLIMS_G2000_A0325.ini file for mixing ratio dependency tests
2017-01-31	Salt liner tests
2017-04-24	Changed N2 supply plumming with separate pressure regulators
2017-08-31	Vapourizer cleaning with warm water
2017 - 10 - 31	Last activity on log for that year



Figure 4: Data availability for the HKDS2039 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

2018-02-20	Instrument reassembled after autosampler has returned
2018-03-16	Instrument moved to GFI tower for water vapour measurements during IGP
2018-03-22	Installed instrument at FARLAB
2018-09-27	Installation on board R/V Kronprins Haakon (AeN)
2018-10-21	Installation at FARLAB
2018-12-18	Installation at GFI tower (SNOWPACE2018)



Figure 5: Data availability for the HKDS2039 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 log for 2019

2019-02-08	Installation at FARLAB
2019-05-07	Vapourizer cleaning
2019-12-20	Installing CWS (continuous water sampler)

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Figure 6: Data availability for the HKDS2039 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	

2020-01-02 to 2020-01-04	CWS testing
2020-01-24	17-O test runs
2020-01-28	Instrument moved to DI lab for microdrop and crusher testing
2020-01-30	Installed python 2.7.17 to enable microdrop script operation
2020-02-05	Microdrop calibration tests
2020-02-11	Instrument back in CF lab

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Figure 7: Data availability for the HKDS2039 during 2020 for (a) JFM (b) AMJ (c) JAS (d) OND.