# Routines for liquid water isotope analysis at FARLAB

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Here we present the central steps in the water isotope analysis at FARLAB, University of Bergen. Here we focus on the routines done to correct data for known biases and problems.

## 1. Analysis procedures

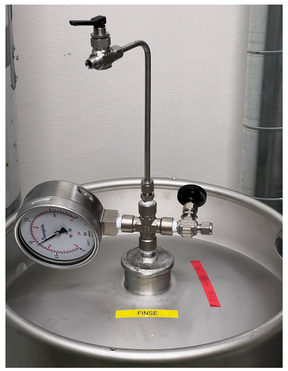
Incoming samples are assigned to an internal project number and registered in a lab-management database. Analysis then proceeds along the following steps:

1. Samples are filtered and transferred to 2 ml GC-vials
2. We use Picarro 2140i spectrometers
3. Typically 10-16 injections are done for every sample, starting with a double injection to “flood” the vaporizer, reducing memory from previous samples
4. The run setup includes typically 4 standards:
   - 2 calibration standards spanning the range of the samples
   - 1 drift standard every 5-6 samples
   - 1 long term control standard
5. Typical run length is 20-30 samples (2 days)

## 2. Run setup

Runs are set up with 4 standards for calibration and drift control. Drift standards allow for quantification of short-term reproducibility and long-term drift.


## 3. Standard storage

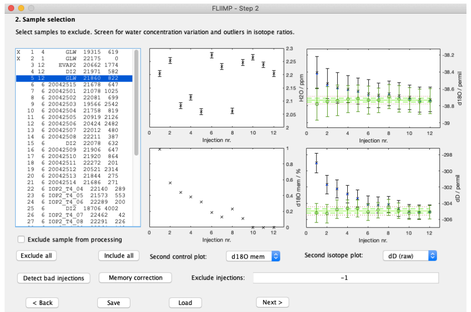


Isotope water standard waters are filtered and stored in 50L stainless steel beverage containers, following IAEA recommendations.

The containers are filled to about 40L and pressurized with up to 1 bar $N_2$. Water can then be tapped through a riser without opening the cask, avoiding diffusive loss.

We work with 5 secondary lab standards at FARLAB: GLW, FIN, DI2, BERM, and EVAP2.

## 4. Processing with FLIIMP



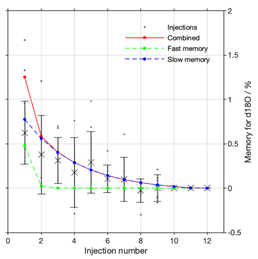

FLIIMP in Version 1.8.1 is the Matlab-based software that we use to process the measurements. It allows automated and manual review of all injections, batch-wise memory correction, drift correction, calibration and uncertainty assessment.

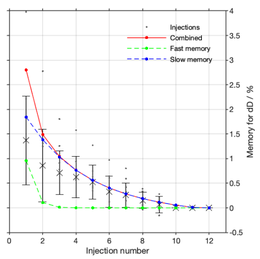
If needed, runs can be re-processed with later versions from a file-system based data storage structure.

## 5. Memory correction

Memory correction is done by combining fast and slow memory estimates based on an exponential fit to the measurements of calibration and drift standards in the current run of the form:

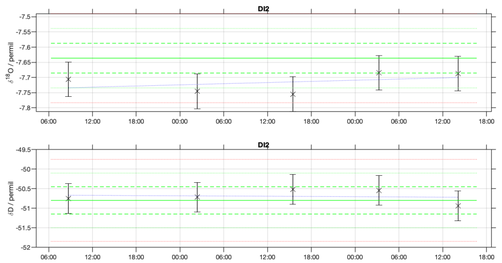
$$M_j = M_0 \left( w \cdot e^{-a \cdot j} + (1 - w) \cdot e^{-b \cdot j} \right)$$



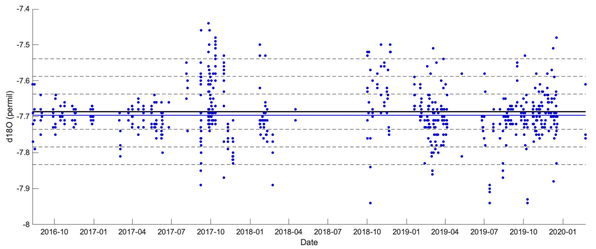

## 6. Drift correction

Drift correction is done by linear regression of the delta values the drift standards against time. Depending on remaining trend and drift offset, individual runs are retained or rejected, resulting in re-measurement of samples.




## 7. Long-term reproducibility

Long-term reproducibility is quantified from calibrated measurements of drift standards in use at FARLAB. During 2016-2020, drift standard DI showed and long-term reproducibility, estimated from the 1-sigma standard deviation as 0.491 permil for δD, and 0.076 permil for δ18O. In 2020, drift standard DI2 replaced DI. Runs with consistent poor drift standard performance (>3 standard deviations) have been excluded from this assessment. Other drift standards result in similar estimates, albeit for shorter time periods.




## 8. Combined uncertainty

FLIIMP calculates the propagated uncertainty of the
- Primary standards
- Secondary standards
- Standard measurements
- Repeated measurement of the samples
- Long-term reproducibility?

following Gröning (2018).

Customers receive standardized reports for each batch of samples explaining the processing steps and the calculation of combined uncertainty.

*Gröning, Manfred, 2018: SICalib User Manual (Stable Isotope Calibration for routine δ-scale measurements) Ver 2.16j, Terrestrial Environment Laboratory, International Atomic Energy Agency, Vienna, Austria

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