DEVELOPMENT OF A PORTABLE MASS SPECTROMETER FOR HYDROLOGICAL APPLICATIONS

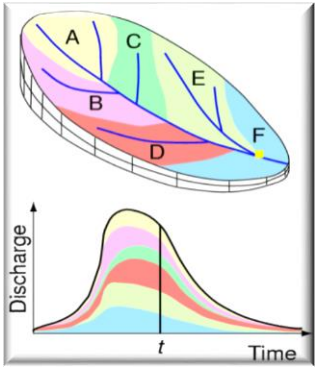
H.Q. Hoang, V. Lopez, D. Dowsett, T. Wirtz,
J.J. McDonnell and L. Pfister

HEMS, Baltimore, 13-16 Sept 2015

LUXEMBOURG
INSTITUTE
OF SCIENCE
AND TECHNOLOGY

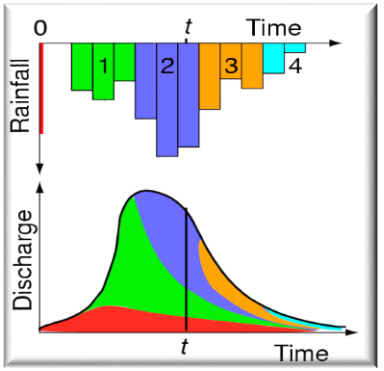
Stable isotopes in hydrology

Geochemical tracers



Spatial origin of water & water flowpaths

Stable isotopes



Catchment transit time & event/ pre-event water separations

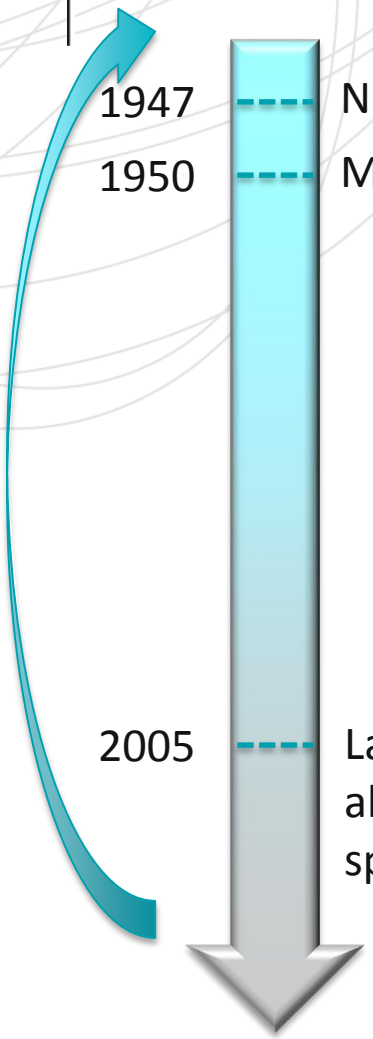
Stable isotopes in hydrology

Grab sampling
(> daily)

Automatic samplers
(event-based,
streamflow triggered,
> 30 minutes)

Need for high-frequency measurements directly from the field

Isotope-ratio measurement techniques in water



1947 Nier MS

1950 McKinney MS

- Infrared spectroscopy
- Freezing point
- Falling drop
- Gas chromatography
- **Mass spectrometry** →

Inert gas as carrier of isotopic signature

- ✓ Accurate
- ✓ Lab-based condition
- ✓ Time consumed

2005 Laser absorption spectroscopy

- **Mass spectrometry**
- **Laser absorption spectroscopy** →

- ✓ Fast
- ✓ Accurate
- ✓ Lab-based condition

Isotope-ratio mass spectrometry in water

Direct injection of water
- ✓ Fast
- ✓ Inaccurate
- ✓ Absorption, recombination

Water molecules react with ions → formation of H_3O^+

Inert gas as carrier of isotopic signature
- ✓ Accurate
- ✓ Lab-based condition
- ✓ Time consumed

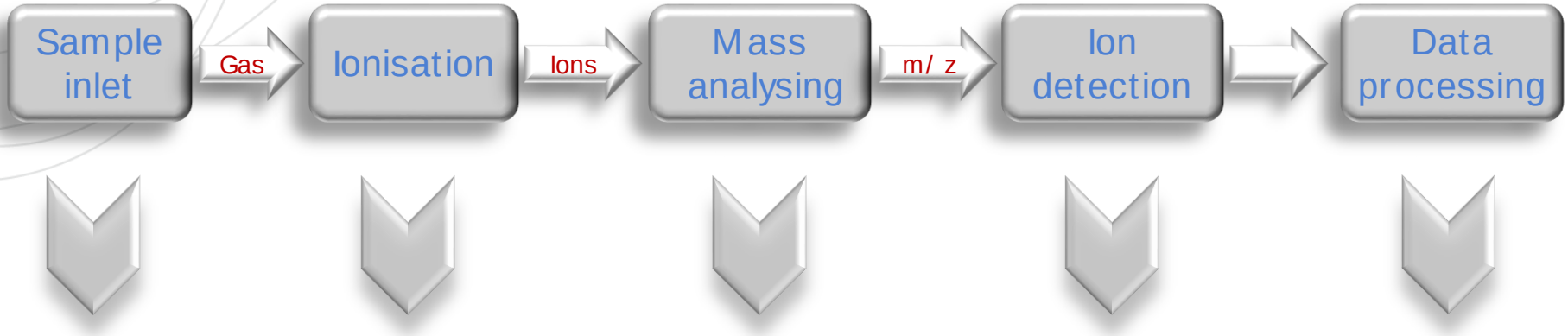
Converting H_2O (liquid) into H_2 (gas) and CO_2 (gas)

Portable mass spectrometer with high measurement frequency but lower precision

Field deployable mass spectrometer for hydrology application

1. Portable
2. Deployable in the field (5-35° C, minimum calibration)
3. High sampling frequency (10-15 minutes)
4. Low energy consumption (<100W, battery life of a few days)
5. Mass resolution $M/\Delta M > 1500$ to eliminate interferences

Instrumental concept



MIMS
-Nafion membrane

Electron impact ionisation (EI source)

Magnetic sector mass analyzer
- Parallel acquisition
- High transmission

Focal plane detector
Slit detector

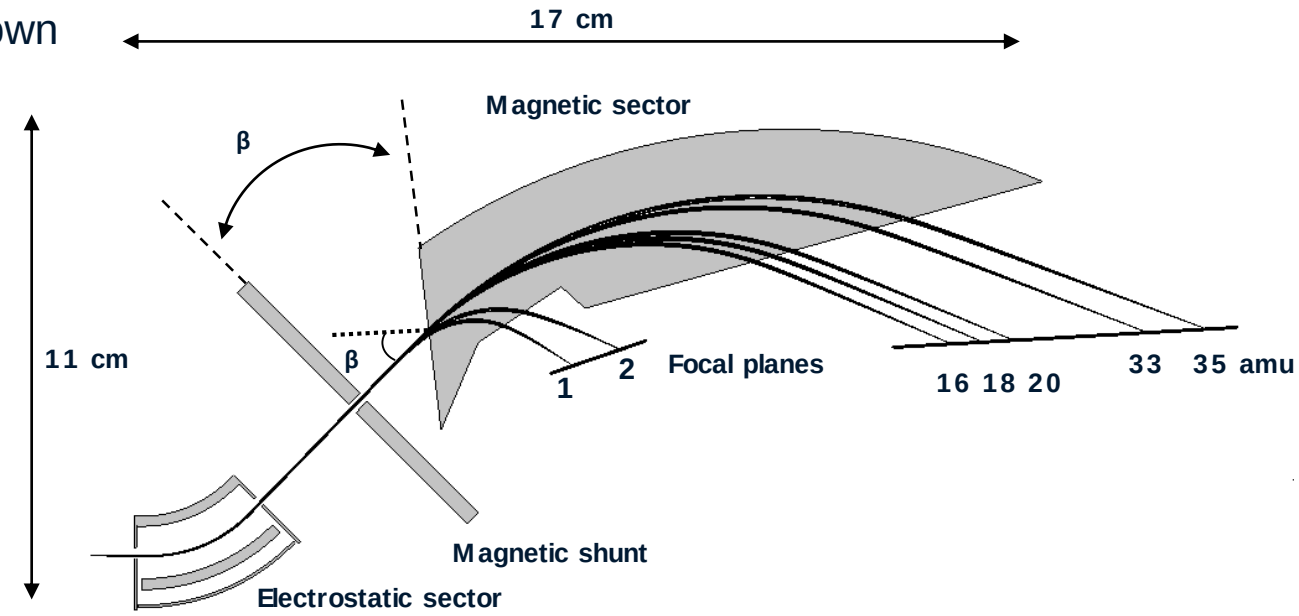
- Interface board
- Control software

A compact mass analyzer design

Schematic layout (ion trajectories in Lorent-3EM)

- ✓ Spherical electrostatic sector
- ✓ Magnetic shunt
- ✓ Magnetic sector
- ✓ Beam energy of 5KV
- ✓ Size of the analyzer

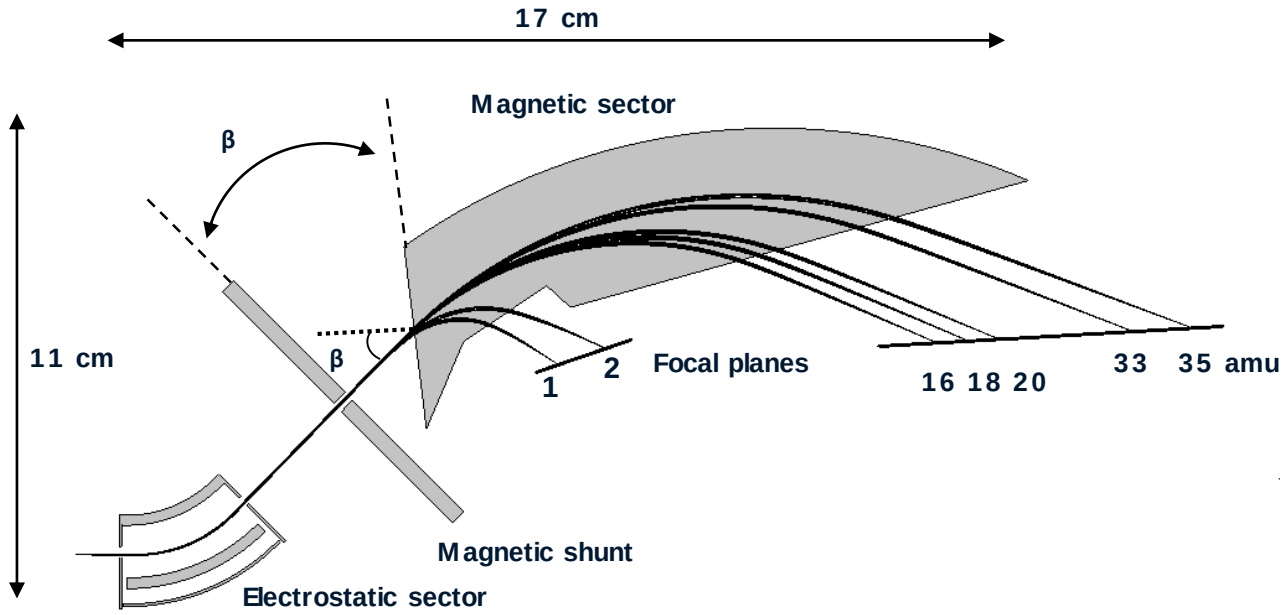
can be scaled up or down



A compact mass analyzer design

Design parameters

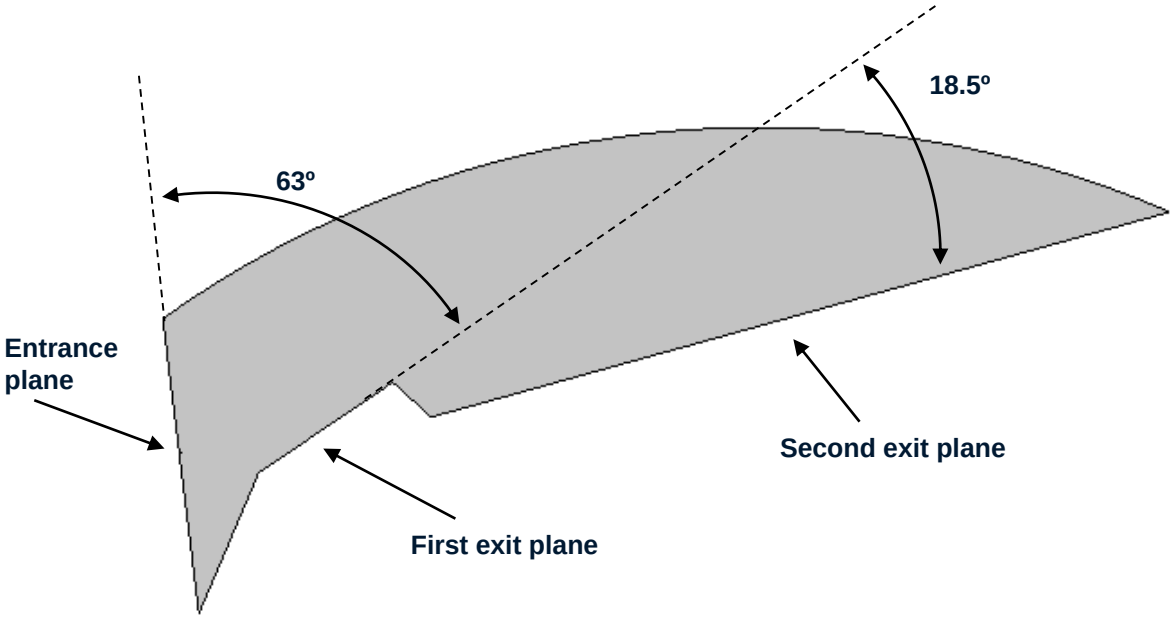
- Magnetic shunt
  - ✓ Inclined angle between the shunt and the magnetic sector
- Magnetic sector
  - ✓ Two different focal planes

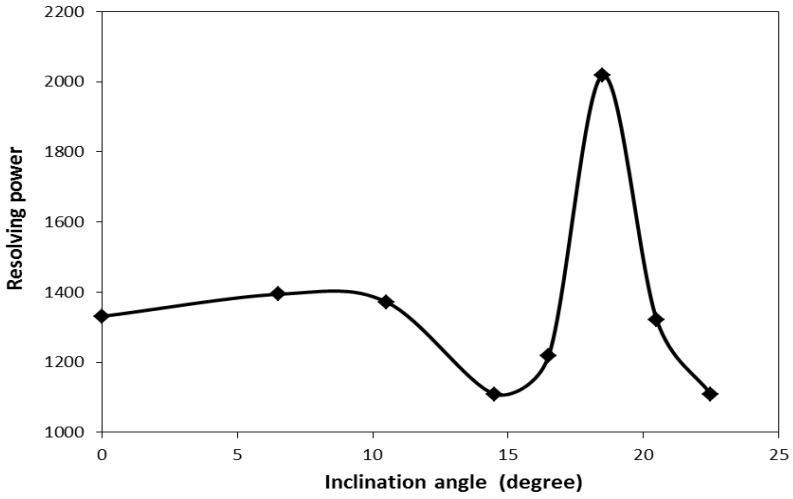


A compact mass analyzer design

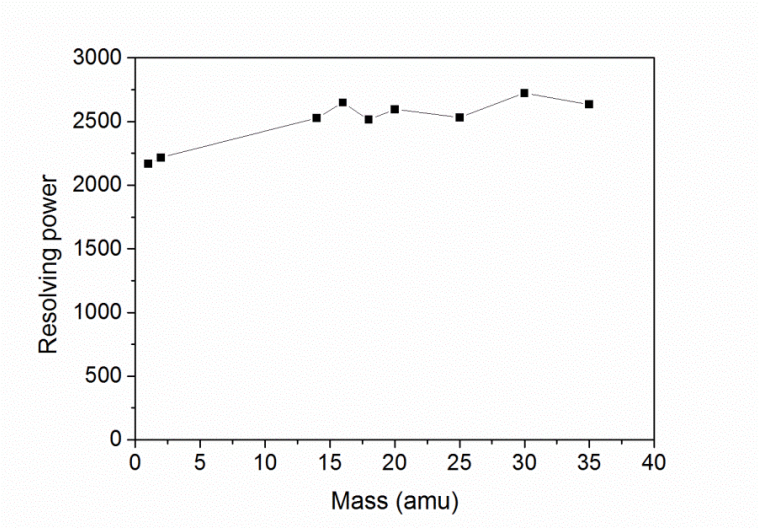
Design parameters

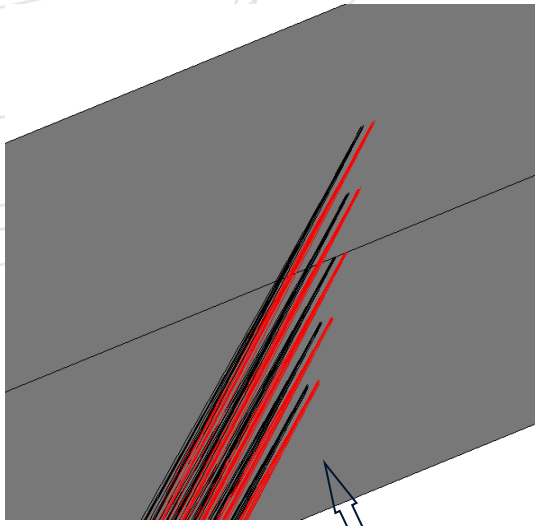
- Magnetic shunt
  - ✓ Inclined angle between the shunt and the magnetic sector
- Magnetic sector°
  - ✓ Two different focal planes

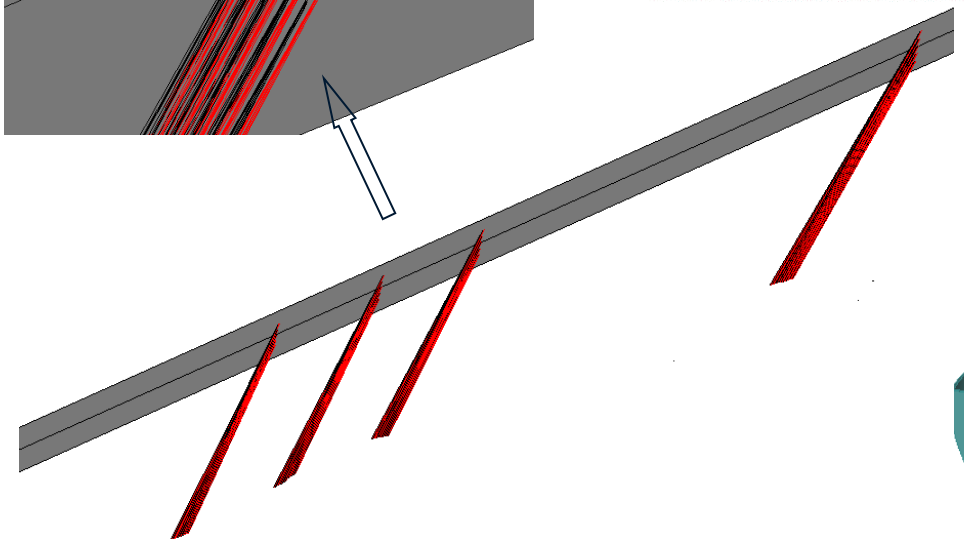


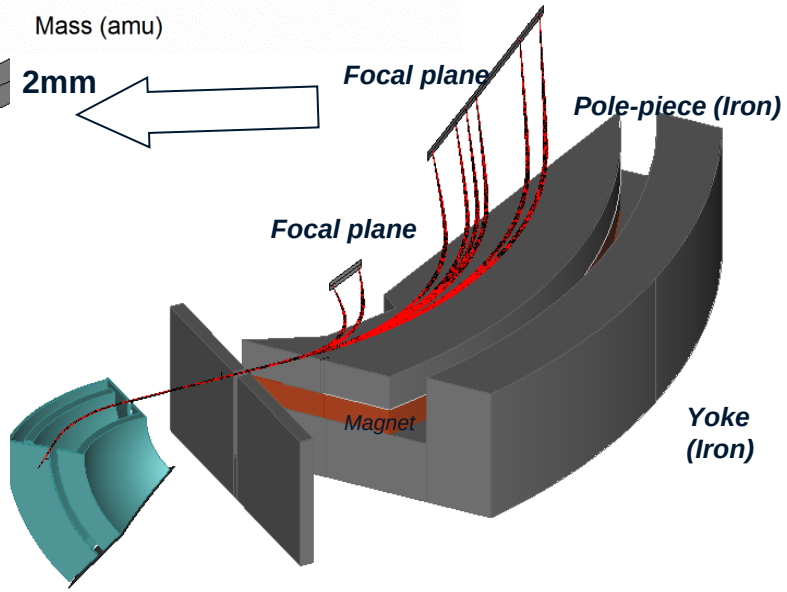


A compact mass analyzer design









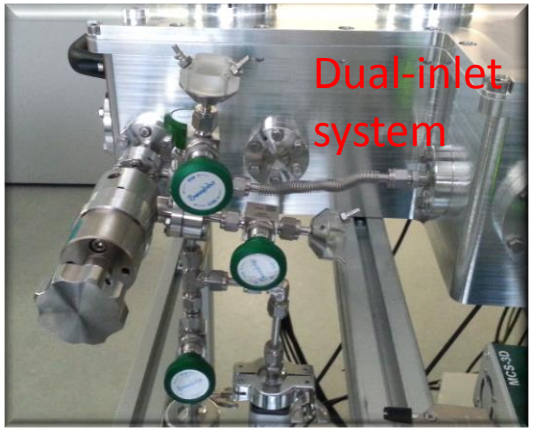
Electrostatic sector

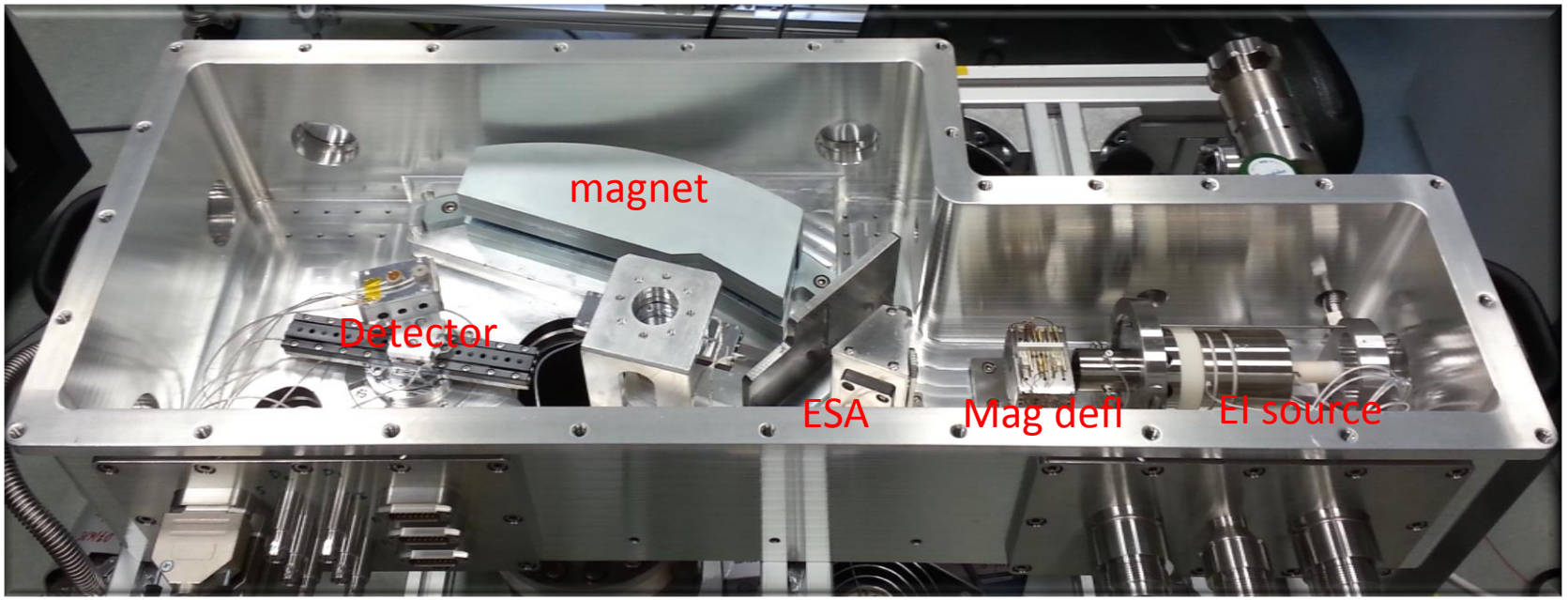
Magnetic shunt

Magnetic sector

Prototype

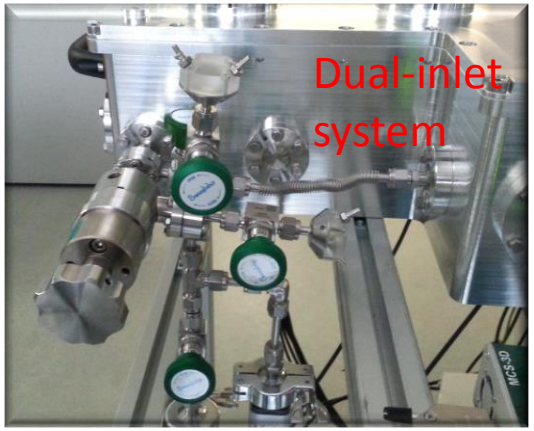
- Detector position adapting to temperature change
- Measurement frequency: 20 mins

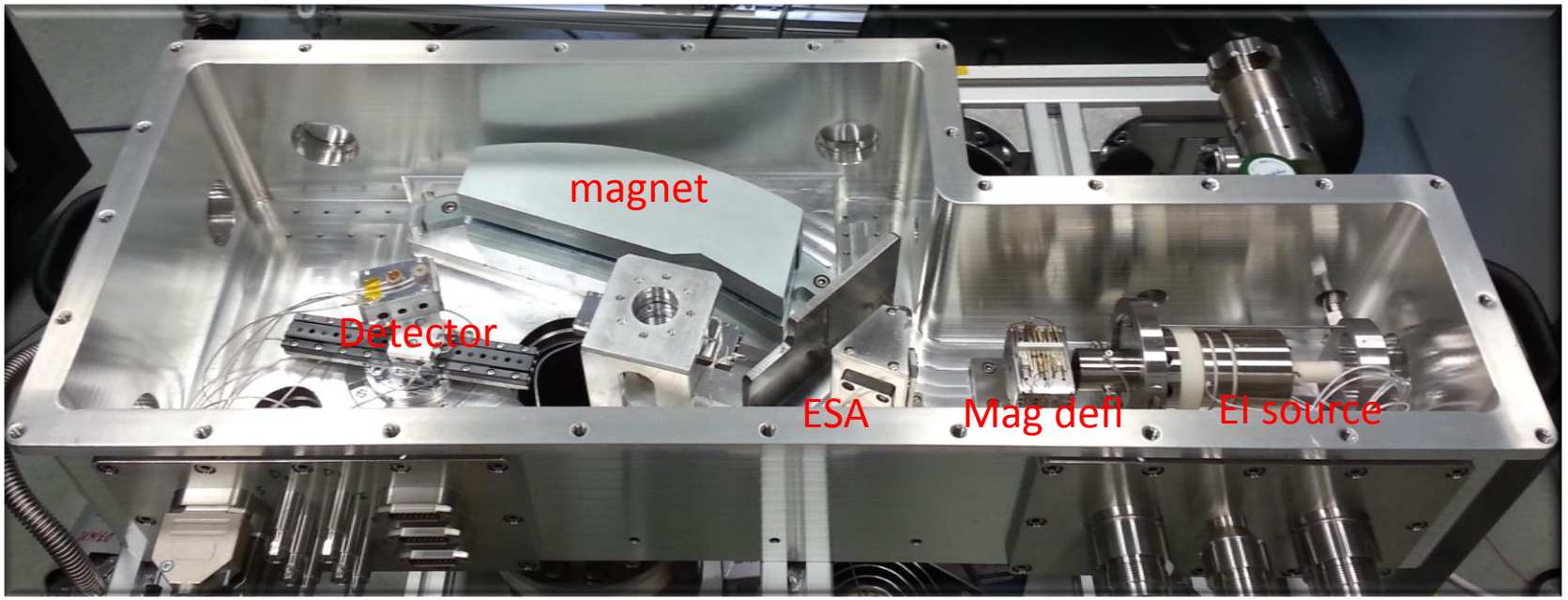




Prototype

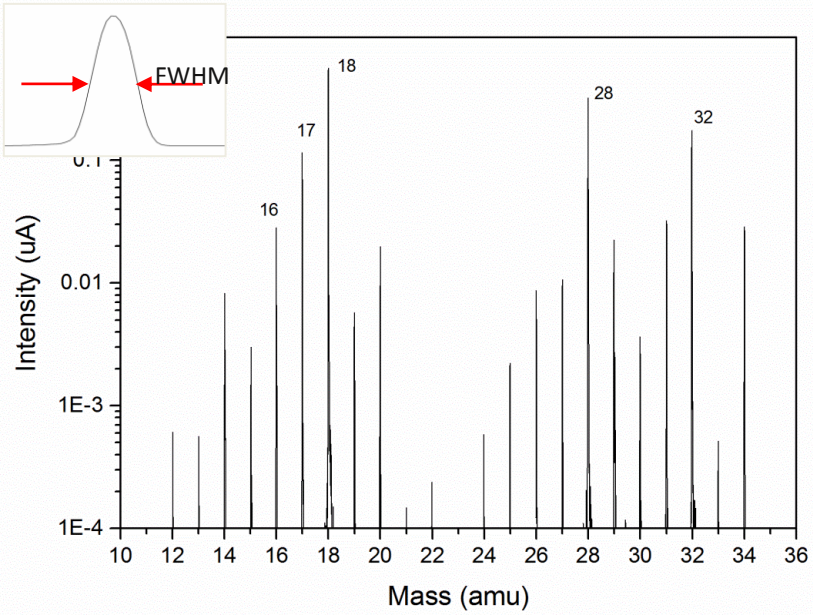
- Size: 72x27x17 cm (only the vacuum box)
- Weight: 50 kg including the pump and electronics



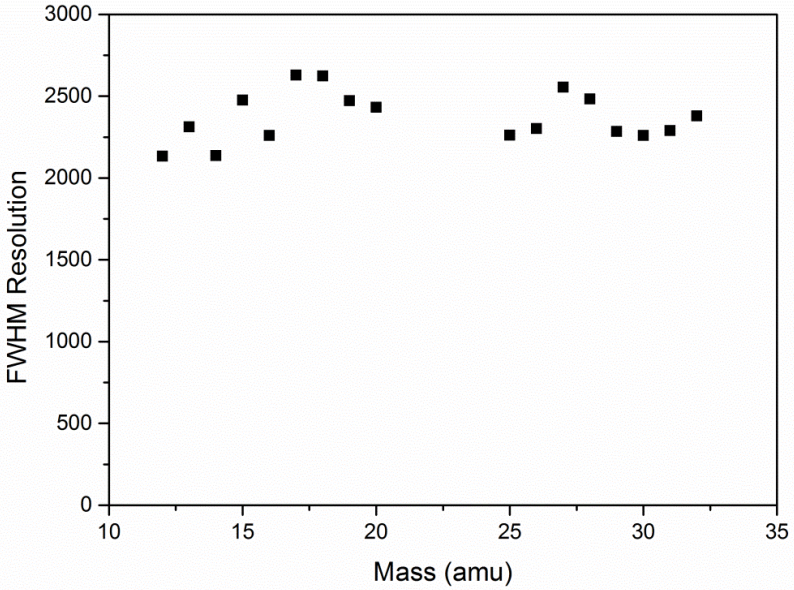


Instrument performance

Mass spectrum of a mixture of ammonia + water + air

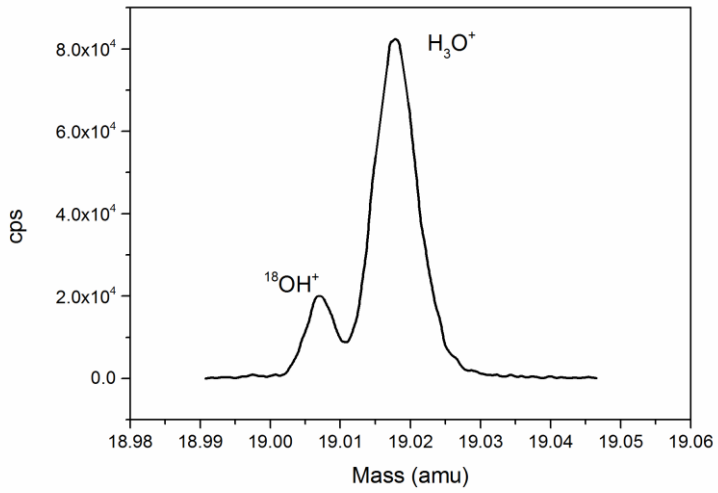


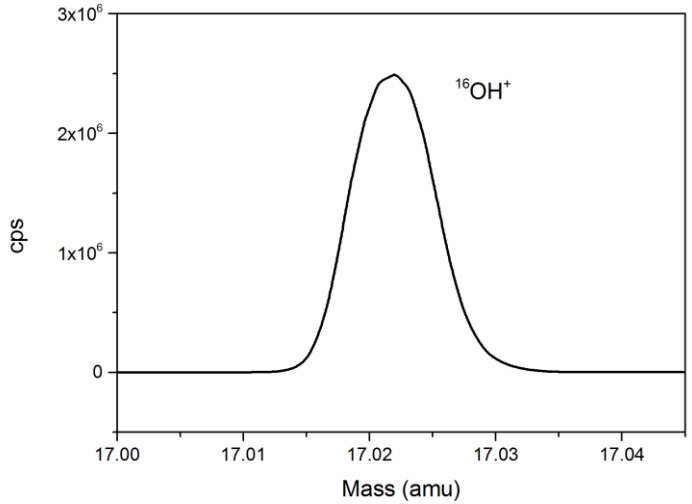
Mass resolving power



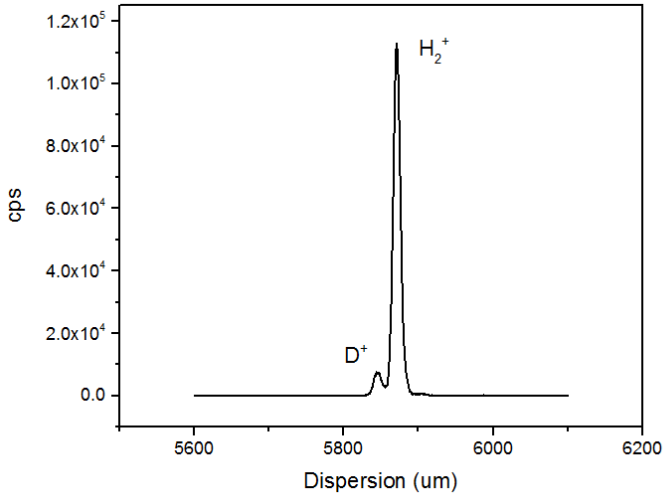
Mass resolving power of above 2000 → enough to resolve $^{18}OH^+$ from H_3O^+ and $^2H^+$ from H_2^+

Isotope ratio measurement





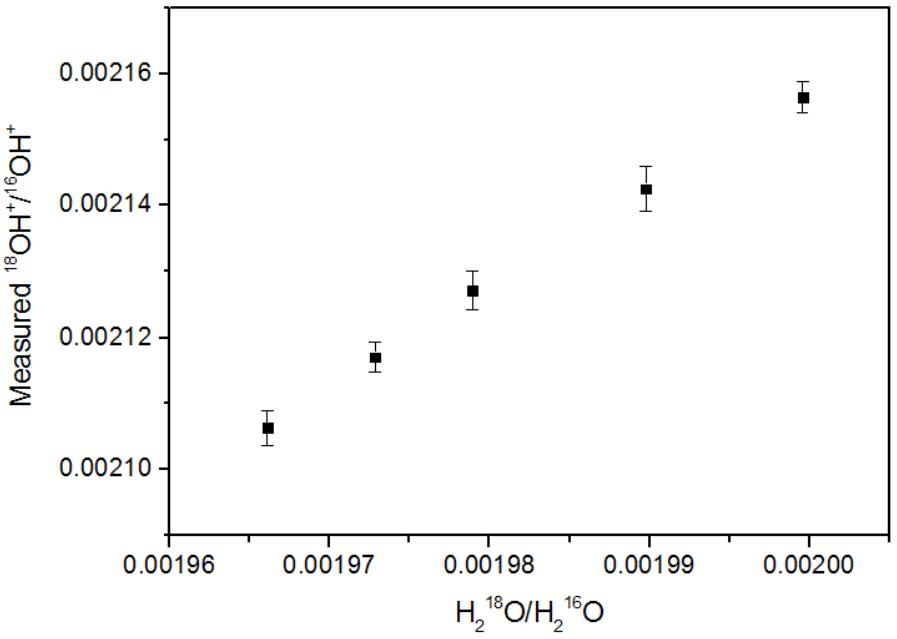
Ratio of $^{18}OH^+$ and $^{16}OH^+$ for isotope ratio of ^{18}O



Ratio of D^+ and H_2^+ for isotope ratio of Deuterium

Isotope ratio measurement

Reproducibility of ^{18}O measurement



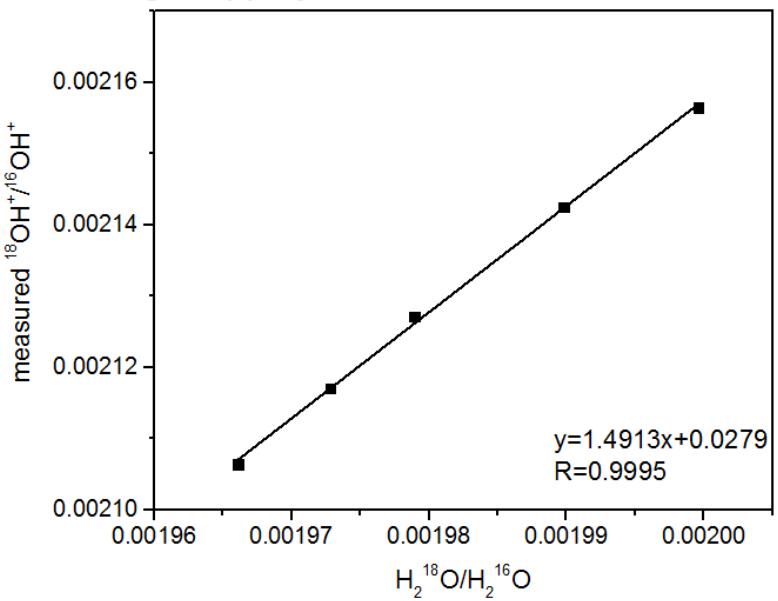
- 5 standard water samples
- 20 measurements for each sample
- Different times with the same ionization current and pressure

→The precision of the measurements varies between 1 to 2.5‰

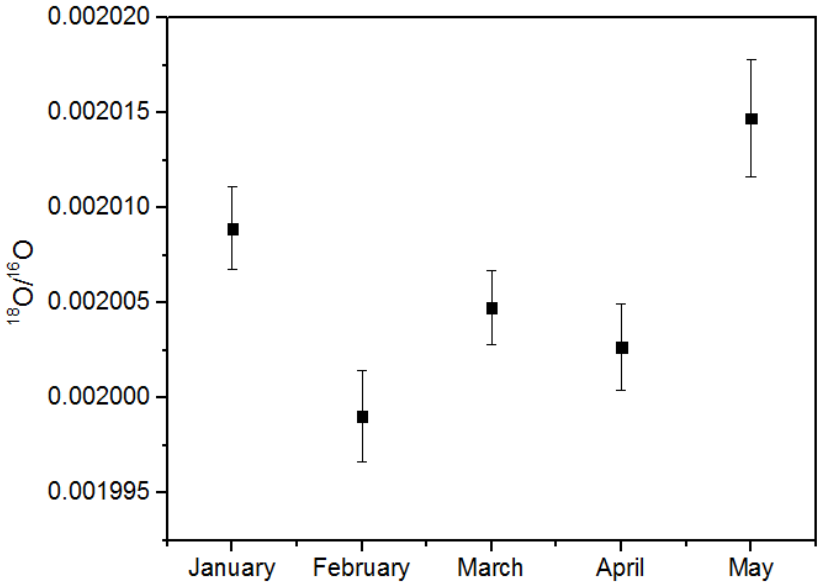
→The precision of the LGR (Los gatos) laser absorption spectrometry instrument in LIST ranges between 0.1-0.8 ‰

Isotope ratio of rainfall samples

Callibration curve

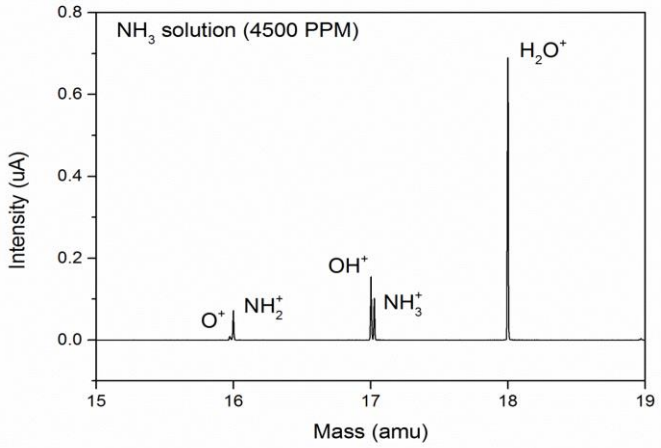


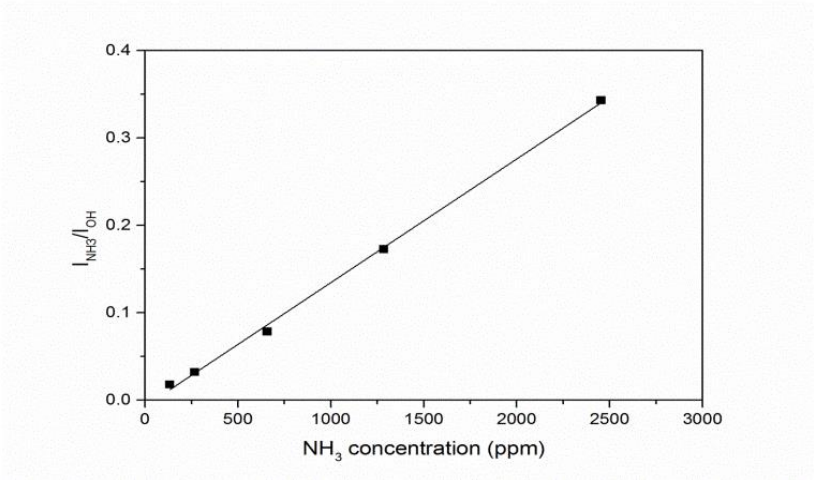
Isotope ratio of rainfall samples

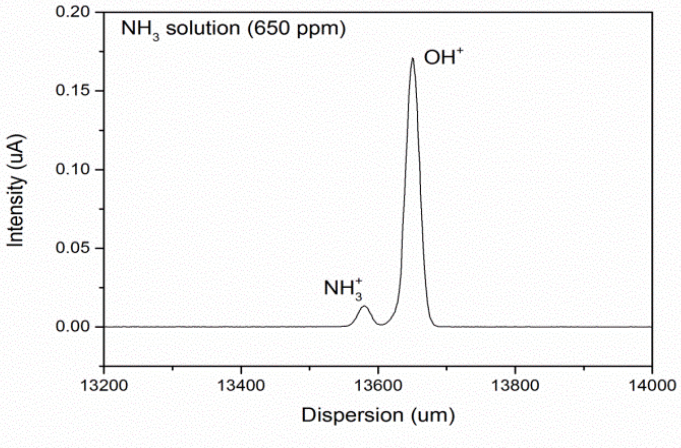


Other applications

- Nitrate in water







- Need to convert nitrate into ammonia (electro-chemical)
- Detection limit of about ppm

LUXEMBOURG INSTITUTE OF SCIENCE AND TECHNOLOGY

Thank you!