ISOARC project

Samoylov water vapour isotopes analyser raw data

Within the ISOARC project, the water vapour analyser on Samoylov is dedicated to the continuous measurements in ambient air of humidity level (in ppm), $\delta^{18}O$ and δD (in permil, ‰).

The raw dataset archived in PANGAEA consists of two types of files, which have to be combined for a correct use of the observations. The description of the files structure is provided thereafter, following explanations about the calibration protocol.

Calibration protocol

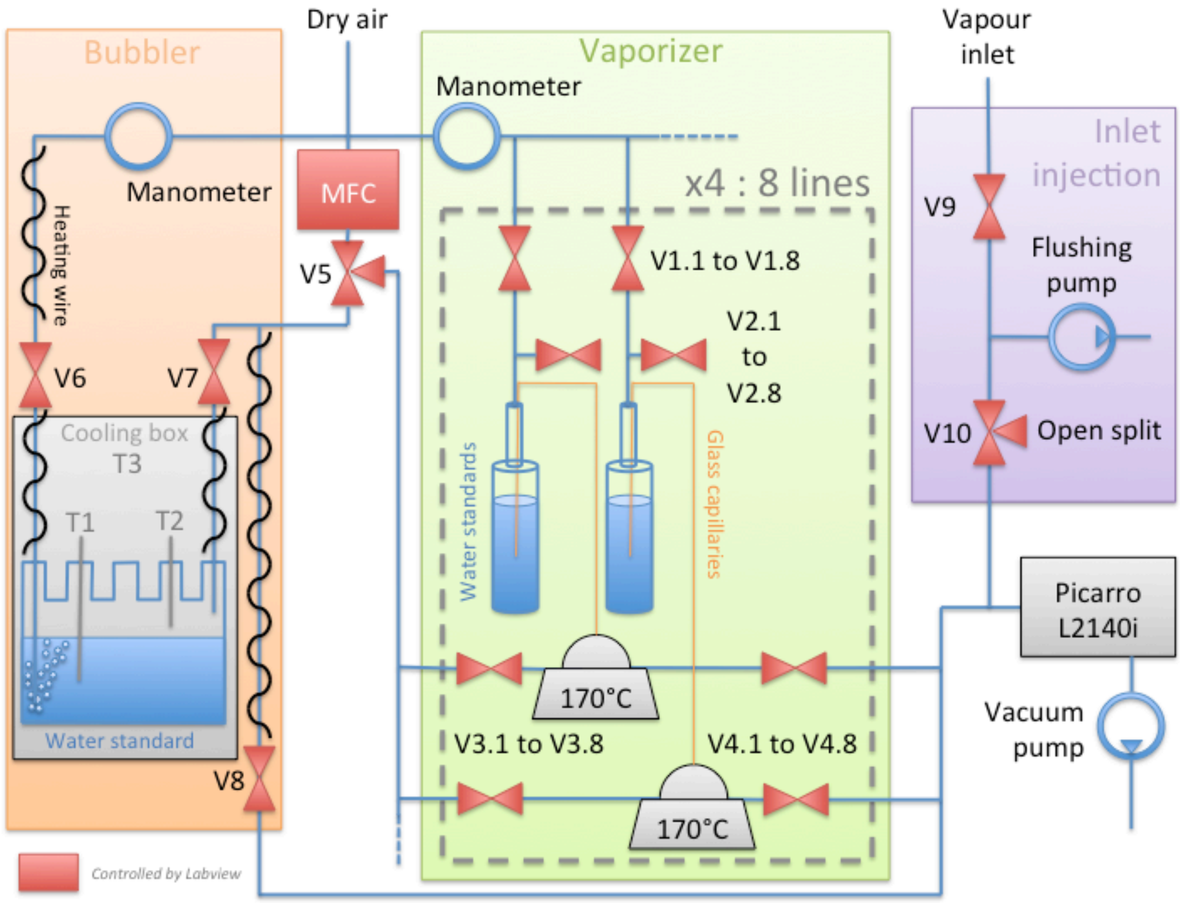

Figure 1: Schematic of the water vapour isotopes analyser calibrations and ambient air injection system.

A schematic of the analyser setup is presented in Figure 1. The analyser is a Picarro brand L2140i Cavity Ring Down Spectrometer, operating with a custom-made calibration system. Ambient air is continuously pumped through a heated tube, with an inlet located at about 5 meters height above ground level. The analyser is continuously measuring and recording data at a frequency of about 1Hz. An injection and calibration system controlled by a Labview program running on an independent computer switches automatically the humidity air sources analysed by the instrument: either ambient air sampled from the inlet or air coming from the calibration unit. The calibration of the instrument consists of the successive injection of water vapour samples with different isotopic compositions independently known. For a better stability of the instrument, two independent calibration systems have been installed on the instrument and are presented hereafter.

The first calibration system, later named vaporizer, consists in vaporizing the water standards at high temperature and mixing them with dry air. It corresponds to the green shadow zone of Fig. 1. Four different standards can be delivered by eight independent lines, two lines being dedicated to each standard for a better resilience of the system. The names of the 8 lines of the vaporizer are successively 1A, 2A, 3A, 4A, 1B, 2B, 3B, and 4B. Each standard should be used both on A and B lines of the same number. The calibration standards are in liquid form, stored in glass bottles, and have to be vaporized before being injected into the analyser. The liquid water is injected through glass capillaries into a tee piece heated at 170,0°C and mixed with dry air coming from a high-pressure gas bottle. Increasing the pressure in the bottles containing the liquid standards (using the air pressure from the gas bottle) allows the standard water to be pushed into the glass capillaries.

The second calibration system, later named bubbler, consists of custom dew point generator providing a humid air of theoretically known isotopic composition. It corresponds to the orange shadow zone of Fig. 1. It allows measurements of only one standard. Dry air is injected under the form of small bubbles through a large amount of this liquid standard under a controlled environment: temperature probes T1 and T2 are respectively recording the water and air temperature inside this bubbler system.

Both calibration systems use dry air, which can be provided either by a dry air generator or by a dry air gas bottle. The instrument is routinely operated with dry air from the dry air generator, but some tests were performed with dry air from a gas bottle. An operating checklist contains the necessary information about the dry air source used.

The different valves shown on fig. 1., controlled by the Labview program, are used to control the injection in the analyser. The inlet injection part of the system, in purple on fig. 1, determines the humidity sources: ambient air inlet, air from the room or air from one of the calibration systems. A pump continuously flushes the air inlet, as long as valve V9 is opened. When the valve V10 is opened, all the vales V4 (V4.1 to V4.8) from the vaporizer and the valve V5 from the bubbler system should be closed, and the flow comes from the ambient air inlet. If both V10 and all the valves V4 and V5 are closed, the air comes from the open split of valve V10, in other words from the room, where the analyser is installed. When one or several of the valves V4 or V5 are opened and the valve V10 is closed, the flow goes from the corresponding calibration systems to the analyser, and the over-pressure is released through the open split.

The vaporizer system is controlled by all the V1 (V1.1 to V1.8), V2 (V2.1 to V2.8), V3 (V3.1 to V3.8) and V4 (V4.1 to V4.8) valves. To inject dry air through the vaporizer, the V5 valve should not be activated. Opening both valves V3 and V4 on one line allows dry air from the gas bottle to be pushed into the system and measured by the Picarro. Opening the valve V1 will pressurize the glass bottle and push liquid standard water through the capillaries towards the oven. On the other hand, opening valve V2 will release the pressure in the bottle. If valves V3 and V2 are opened at the same time on one line, liquid water and then dry air will be pushed back into the bottles (this purge is more efficient when V4 is closed). This last combination is used to dry the lines and avoid accumulation of water after the injection of water.

The bubbler system is controlled by all the valves V5, V6, V7 and V8. A heating wire can also be activated while using the bubbler to warm the incoming and out coming air to prevent condensation in the calibration system. Activating V5 and V8 will allow dry air to be directed through the outlet of the bubbler system towards the analyser. Activating V7 will allow the dilution of wet air coming from the bubbler by dry air. Activating V6 will inject dry air through the bubbler itself and thus provide wet air. Three temperature values are measured: T1, T2 and T3, which respectively correspond to the temperatures from the liquid water standard, from the air inside the bubbler and from the cooling box in which the bubbler is placed.

Here is a summary of the main open valves combinations used for the different injections (assuming that all other valves are closed):
Vaporizer control:
- V1, V3, V4: Injection of vaporized standard in the system and measurement.
- V3, V4: Injection of dry air in the system and the Picarro analyser. Used to dry the lines
- V2, V3: Push back water and dry air into the bottles.
- V2, V3, V4: Push back water and dry air into the bottles and the Picarro analyser.
- V2: Release pressure in the bottles
Bubbler control:
- V5, V6, V7, V8: Injection of wet air from the bubbler in the system and measurement.
- V5, V8 or V5, V7, V8: Injection of dry air in the bubbler outlet and the Picarro analyser. Used to dry the line
Choice of air source:
- V9, V10: ambient air measured
- V9, V4: air from the vaporizer measured, over-pressure released through open split
- V9: room air through open split

The humidity level of the calibration can be regulated by two mains: (i) changing the dilution with dry air by adjusting the flow of dry air via the Mass Flow Meter (MFC) controlled by the Labview program (an higher dry air flow giving lower humidity levels), or (ii) adjusting one of the manual manometers to regulate either the pressure applied into the bottles containing the liquid water standards for the vaporizer (a higher pressure giving a larger water flow and thus higher humidity levels) or the flow of dry air pushed into the bubbler for the bubbler system.

Typical valve control sequences used during routine measurements last 25 hours and consist of the successive injections of each calibration standard during 30 minutes, surrounded by a purge of the lines with dry air for 2 minutes, and followed by the injection of ambient air from the inlet system. Either both calibration systems are used successively, or only one is used for the normal calibration sequence. A manual control of the system is also possible with the Labview program, and is mainly used during the maintenance periods of the analyser.

To calibrate the instrument regarding its dependency to humidity level, experiments are performed approximately twice a year: each standard is injected at different humidity levels covering the range of humidity values expected for ambient air observations.

During those experiments, the standards are injected several hours, and the humidity levels are changed every 30 minutes by adjusting the MFC command voltage. To cover the full range of expected humidity values, both adjustments of the MFC and the manual manometers are needed. Thus, several sequences covering the full MFC range are usually performed with different pressures in the water samples bottles.

Data files structure

The dataset generated by the analyser setup is composed of two different types of files, which must be combined for a correct use of the data: files from the Picarro analyser containing the raw measurements of humidity and its isotopes, described in subsection a, and files from the Labview program containing the information on the applied different valve settings, described in subsection b.

The computers clocks are normally synchronised automatically via the network since mid-April 2016. The time zone used is always UTC+00.

a) The names of the Picarro data files follow this nomenclature:
HKDS2021-**YYYYMMDD-HHMMSS**Z-DataLog_User.dat.gz
The date and time in the filenames correspond to the moment of creation of the file. A new file is created every day at midnight and also each time the instrument is restarted (one can also create a new file manually on the Picarro analyser program).
Those files have been compressed using gzip on a Windows computer. When uncompressed, the file extension is *.dat. These are simple text files, containing a header with explicit labels at the first line and 65 columns separated by tabulations. After this label, each line corresponds to one measurement, at a frequency close to 1Hz.

Among other instrumental parameters, the **DATE**, **TIME** give the date and time of each recorded data, under the format YYYY-MM-DD HH:MM:SS.sss. The **H2O**, **Delta_18_16**, **Delta_D_H**, **D_Excess**, **Delta_17_16** and **Excess_17** respectively give the specific humidity (in ppm) and the $\delta^{18}O$, δD, d-excess, $\delta^{17}O$ and ^{17}O-excess values in permil.

b) The names of the files created by the Labview program, named logfiles, are under the form:
LogFile-**YYYYMMDD**.txt
There is one file by day, which contains all the daily available data. The date in the file name corresponds to the date of the data contained in the file. The data are stored at a minute frequency. The columns are separated by tabulations.

The comprehensive labels and descriptions of each column are given thereafter:
Date; time; cal_sys; l1_a_b; l2_a_b; l3_a_b; l4_a_b; l1_v1; l1_v2; 1_v3; l1_v4; l2_v1; l2_v2; l2_v3; l2_v4; l3_v1; l3_v2; l3_v3; l3_v4; l4_v1; l4_v2; l4_v3; l4_v4; l5_v1; l5_v2; 5_v3; l5_v4; l6_v1; l6_v2; l6_v3; l6_v4; l7_v1; l7_v2; l7_v3; l7_v4; l8_v1; l8_v2; l8_v3; l8_v4; s_1; s_2; s_3; s_4; s_5; s_6; in_v9; in_v10; t1; t2; t3; p_date; p_time; h2o; d18o; dhdo
After 20160414 at 00:50:49, it has been a little modified to:
Date; time; vaporizer; bubbler; l1_a_b; l2_a_b; l3_a_b; l4_a_b; l1_v1; l1_v2; 1_v3; l1_v4; l2_v1; l2_v2; l2_v3; l2_v4; l3_v1; l3_v2; l3_v3; l3_v4; l4_v1; l4_v2; l4_v3; l4_v4; l5_v1; l5_v2; 5_v3; l5_v4; l6_v1; l6_v2; l6_v3; l6_v4; l7_v1; l7_v2; l7_v3; l7_v4; l8_v1;

l8_v2; l8_v3; l8_v4; v5; v6; v7; v8; s_5; heat; in_v9; in_v10; t1; t2; t3; p_date; p_time; h2o; d18o; dhdo

- The columns **Date** and **time** correspond to the date and time from the computer running the Labview program controlling the instrument, which is the reference time for the valves switching.

- The **cal_sys** column informs of which calibration system is used: either V for vaporizer or B for bubbler. The vaporizer and bubbler column which replace it after 20160414 at 00:50:49 describe if respectively the vaporizer or the bubbler are activated. The values are respectively V or B if the systems are activated, or X if they are not.

- The next 44 columns correspond to the state of the calibration and inlet injection system. The four columns **l1_a_b**, **l2_a_b**, **l3_a_b** and **l4_a_b** indicate which of the A or B lines from the vaporizer are used for each standard, respectively from line 1 to 4. The possible values are: *-1* for line A, *1* for line B, or *0* if none of the lines are used. The next 32 columns give the state of the 4 valves from V1 to V4 on the 8 different lines, with the nomenclature **l*i*_v*j***, where ***i*** is the line number and ***j*** is the valve number. The values are *0* for a closed valve, and *1* for an opened valve. The columns **v5, v6, v7 and v8** indicate respectively if the valves V5, V6, V7 and V8 from the bubbler system are activated. The values are *0* for a closed valve, and *1* for an opened valve. The columns s_***5*** give the sate of an additional switch. Those switches have been implemented for a potential future enhancement of the instrument, but they have not been used within the system, so far. The column **heat** indicates if the heating wire from the bubbler system is activated. The values are *0* if and *1* if active. The columns **in_v9** and **in_v10** give the state of the two inlet valves respectively V9 and V10, shown in fig. 1. The values are *0* for a closed valve, and *1* for an opened valve.

- The next 3 columns t1, t2 and t3 give the 3 temperature values measured in the bubbler system, respectively the temperatures from the liquid water standard, from the air inside the bubbler and from the cooling box.

- The Labview program imports the last Picarro analyser data every minute from the network connection, and some of those data are saved in the logfile for the synchronisation of both data files. This constitutes the next 5 columns: **p_date** and **p_time** correspond to the Picarro analyser date and time, whereas **h2o**, **d18o** and **dhdo** respectively correspond to the recorded H_2O in ppm and $\delta^{18}O$ and δD values, both expressed in permil. If for some reason, the Picarro data are not imported (for example if the instrument is not recording, if a new Picarro file has just been created after midnight, or if there is a trouble on the network communication between both computers), the corresponding columns will contain the following values: XXXXXXXXXX XXXXXXXX -9999.99 -9999.99 -9999.99

Complementary data

The real values of the standards used on the instrument are measured independently in the laboratory twice a year. These values and the positions of each standard on the different lines are stored in separate files available on https://sensor.awi.de/.

Scientists on-board fill in a checking list (in form of an Excel sheet) on a daily basis, containing a list of parameters checked manually and potential comments during maintenance of the system. This file is also available on https://sensor.awi.de/.