ISOARC project

Polarstern water vapour isotopes analyser raw data

Within the ISOARC project, the water vapour analyser on-board of Polarstern 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 Pangea 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

A schematic of the analyser setup is presented in Figure 1. The Picarro 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.
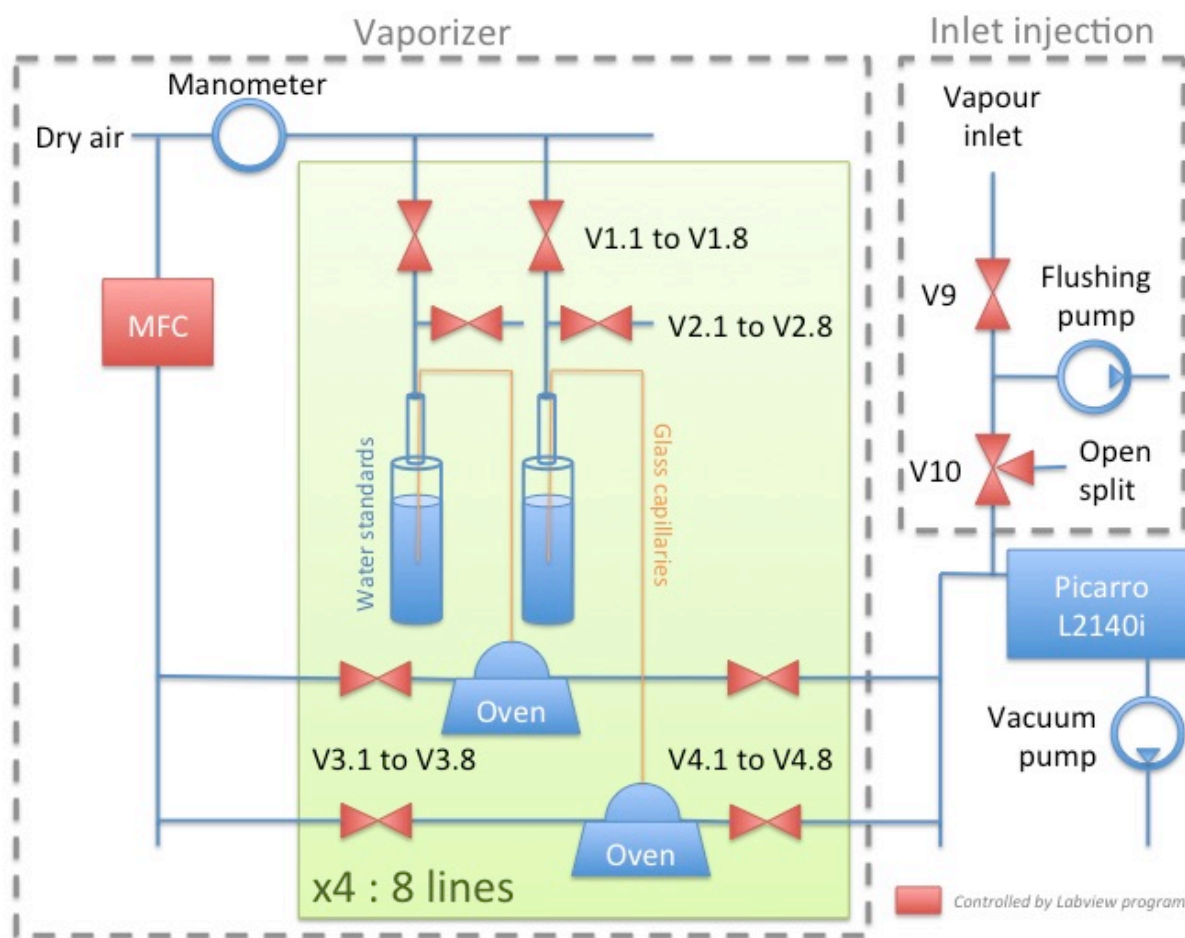

Figure 1: Schematic of the water vapour isotopes analyser calibrations and ambient air injection system.

The calibration of the instrument consists of the successive injection of water vapour samples with different isotopic compositions independently known. This injection is

performed by the system named vaporizer, presented on the left side 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 different valves shown on fig. 1., controlled by the Labview program, determine the use of the different lines. 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 inlet injection part of the system, on the right side of fig. 1, determines the humidity sources: ambient air inlet, air from the room or air from the vaporizer system. 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 should be closed, and the flow comes from the ambient air inlet. If both V10 and all the valves V4 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 are opened and the valve V10 is closed, the flow goes from the vaporizer calibration system to the analyser, and the over-pressure is released through the open split.

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
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) 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 the pressure applied into the bottles containing the liquid water standards with the manual manometer (a higher pressure giving a larger water flow and thus higher humidity levels).

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. 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 manometer 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 via the Polarstern internal network on 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; 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; The p_date; p_time; h2o; d18o; dhdo; lat; N_S; lon; E_W; WS; WD; rWS; rWD; T

- 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 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** indicates which of the A or B lines 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 **li_vj**, 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 s_**k** give the sate of 6 additional switches, where **k** is the number of the 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 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 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 XXXXXXX   -9999.99   -9999.99   -9999.99

- The next columns correspond to the meteorological data imported from the Polarstern DSHIP system. These columns were added to the logfile on the 2015-10-23 at 12:36:19. Thus, those columns do not exist in the logfiles before this date. During the isotope humidity response function experiments, those data are also not imported and there are then no such columns.
The parameters **lat** and **N_S** respectively give the latitude of Polarstern in degree and the hemisphere with the values *N* or *S* for North and South. The parameters **lon** and **E_W** respectively give the longitude in degree and the hemisphere with the values *E* or *W* for East and West. The parameter **WS** and **WD** respectively correspond the absolute wind speed in m/s and the wind direction in degree, whereas the parameters **rWS** and **rWD** correspond to the wind speed and wind direction relative to Polarstern in the same units. The parameter **T** gives the temperature in degree Celsius.
If for some reason the DSHIP data are not imported, the corresponding columns will contain these values:
-999.99 N -999.99 E -999.99 -999.99 -999.99 -999.99 -999.99

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 available in separate files upon request.

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 upon request.