Creation of output spreadsheets

Script functions on the premise that input files' 1st sheet contains the data, and the 2nd sheet contains information about the standards. See *Preparing input files*

Start with sample results

- Replace CH_4 FID values with CH_4 TCD values when CH_4 FID > 50 000 or CH4 FID = 0

Get the N_2O calibrants

- From the first 50 rows of data, select the first 2 non-zero instances of each calibration's N_2O area and calculate the mean

Assign flags to N_2O calibrants (see *Flags*)

Fit linear models using the N_2O calibrants

- 0.98 model includes all calibrants up to and including the 0.98 ppm calibrant
- 80 model includes all calibrants up to and including the 80 ppm calibrant (does NOT include the 9.52 ppm calibrant)

$$Model\ equation = N_2O\ area + (N_2O\ area)^2$$

The 9.52 model is not used and the 9.52 ppm area is not used in fitting the 80 model because of an issue with the 9.52 ppm standard

Calculate N_2O values using the linear models

- Use the 0.98 model's N_2O values when the N_2O values calculated using the 0.98 model are less than 5
- Otherwise, use the N_2O values calculated using the 80 model

Adjust sample data (ie. exclude standards and lab air) to account for dry air instrument standards

$$x_{corrected} = \left(\frac{x}{10^6}\right) * \frac{1 - p_{H2O}}{101.325} * 10^6$$

where $p_{H2O} = \exp\left(24.4543 - 67.4509 * \left(\frac{100}{T}\right) - 4.8489 * \log\left(\frac{T}{100}\right)\right) * 101.325$ is the partial pressure of water at lab temperature converted to kPa

where $T = 20 + 273.15$ is the lab temperature in K

Store one output spreadsheet for each input spreadsheet in the output folder, where each spreadsheet contains:

- all calibrated data
- corrected sample data
- standards (with flags) used in model fitting

Preparing input files

The standards sheet

To process any file, you must create an additional sheet within that file. This is to account for differences in the naming of standards and to ensure that the tool correctly identifies standards.

This sheet must identify all standards within the run such that the standards can be used to fit the N_2O models and to remove all standards from the wet air corrected values.

Requirements

- Contains two columns:
  - RUNINFO
    - Tells the tool which rows contain the standards
    - This should be directly copy pasted from the GC output RUNINFO column
  - STANDARD
    - Tells the tool which standard is being identified
    - If the standard is an N_2O standard, expected values are:
      - 0.1
      - 0.317 or 0.3171
      - 0.69 or 0.696
      - 0.98 or 0.989
      - 9.52
      - 80
    - If the standard is not an N_2O standard (for example, the standard is a CH_4 standard) and should be removed from the wet air corrected data, you may assign any value in this column as long as it is NOT one of the standard ppm values associated with N_2O
- Is the second sheet in the GC excel file to be processed

Example

RUNINFO	STANDARD
N2O 0.1 PPM	0.1
N2O 0.3171 PPM	0.3171
N2O 0.696 PPM	0.696
N2O 0.98 PPM	0.98
N2O 9.52 PPM	9.52
N2O 80 PPM	80
check N2O 0.1 PPM	0.1
check N2O 80 PPM	80
CH4 500	500

Flags

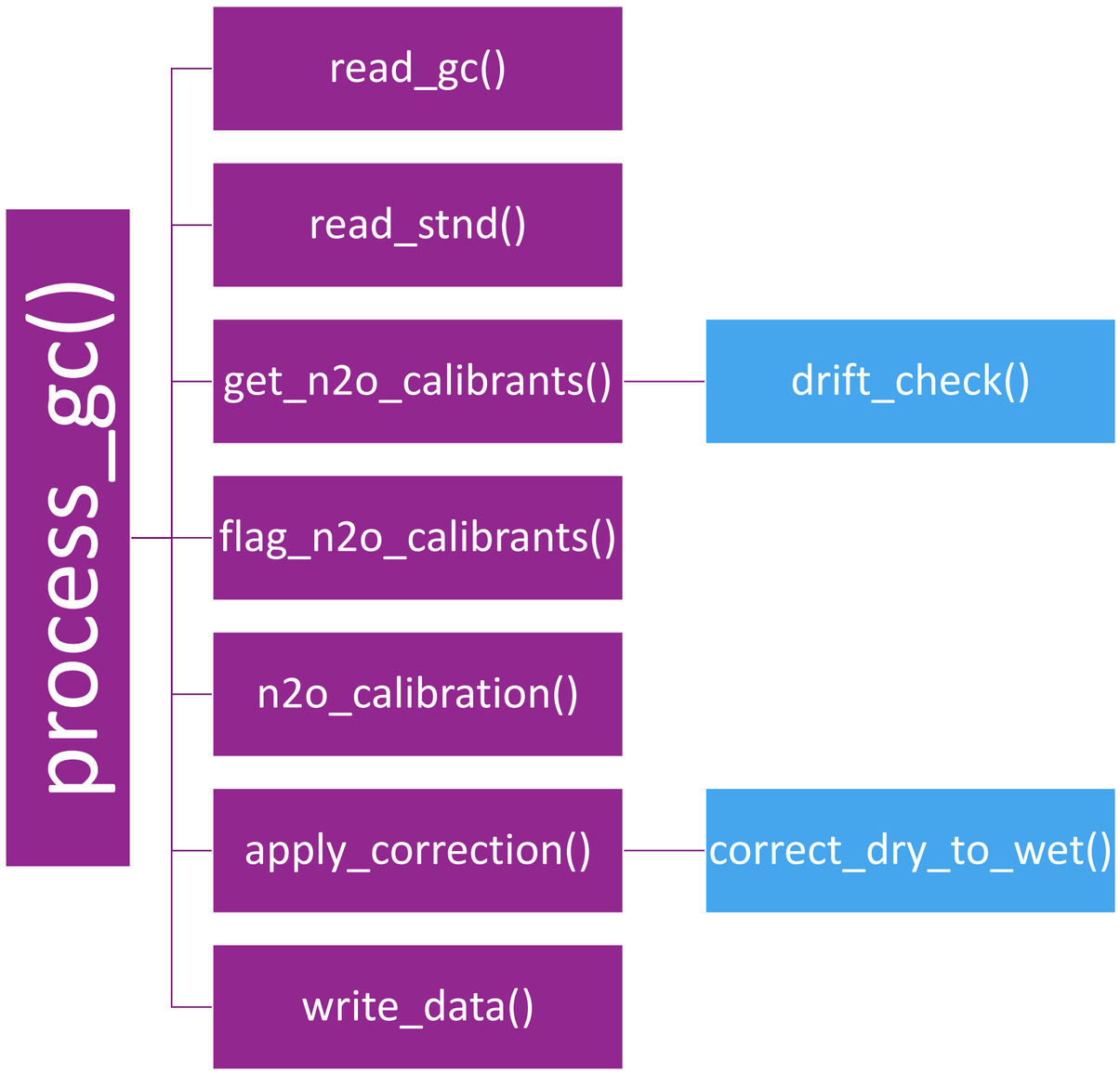
Flags for N_2O standards
used to fit the models

Flag	Meaning
All areas are zero	All runs associated with this standard return a 0 N_2O area
One non-zero area	Only one run associated with this standard returns a non-zero N_2O area
Low N_2O reproducibility (percent difference: #)	Standard returns two permissible N_2O areas with a percent difference > 10%
Standard was not run	No runs associated with this standard were identified

Recall that only the standards in the first 50 rows are used to fit each model

Callstack

For those who need to go into the code



Note that the code to use the 9.52 ppm standard is included in the scripts and will need editing if the standard is to be used

function defined in sc_functions.R

function defined in sc_helper_functions.R