Creation of output spreadsheets

Script functions on the premise that input files' 1st sheet is that one of interest

Start with sample results

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

Get the N_2O calibrants

- Identify if the high standard was 80 ppm or 9.52 ppm by looking for IDs that contain both the keywords "high" and "9.52"
- Select the first 2 non-zero instances of each calibration's N_2O area and calculate the mean
- Determine the mean N_2O area for each calibrant

Calibrants are:
0.1 (low)
0.317 (ref)
0.69, 0.696
0.98, 0.989
9.52
80 (often high, but not always)

Used to identify which standard are associated with "High" IDs that do not contain the associated ppm

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 calculated and the 9.52 ppm area is not used in 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 <= 1
- Otherwise, use the 80 model's N_2O values

Store one output spreadsheet for each input spreadsheet

Flags

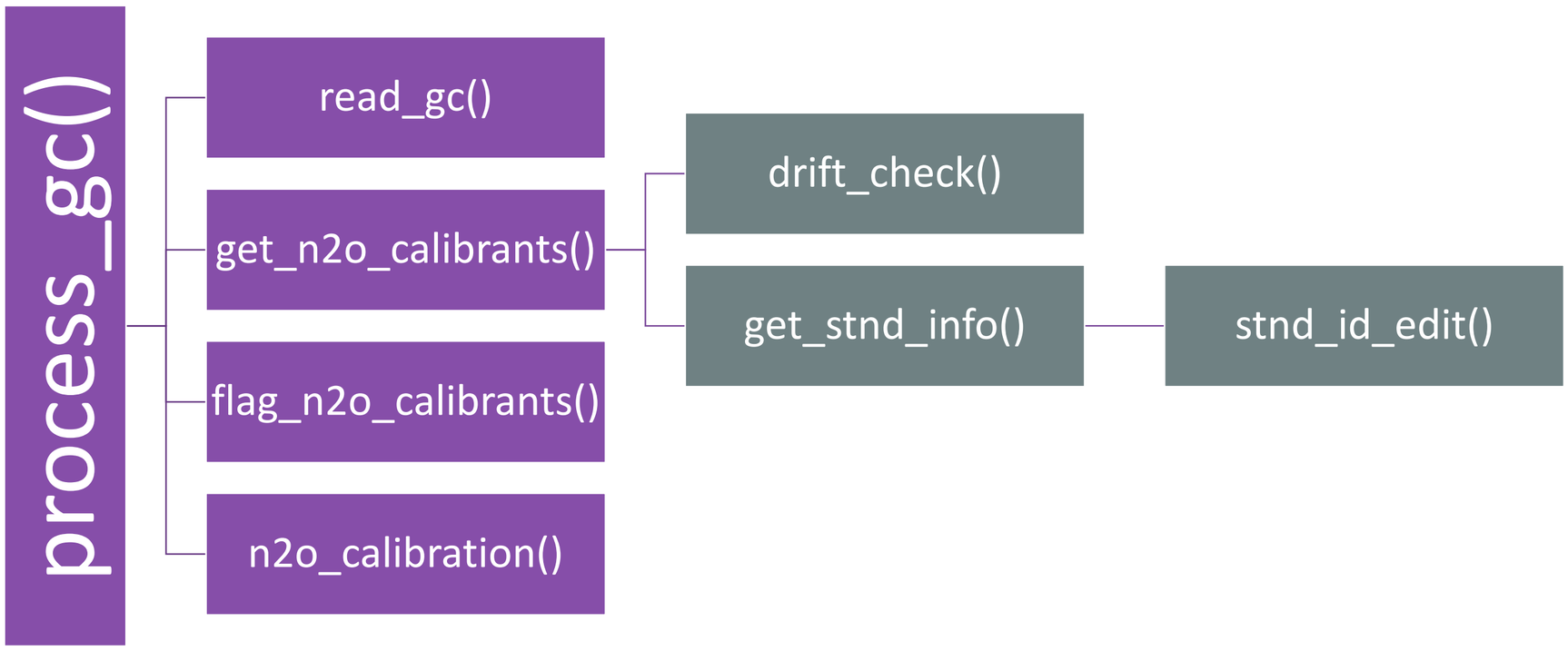
Flags for N_2O standards

Flag	Meaning
All areas are zero	All runs associated with this standard returns 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: #)	When standard returns two permissible N_2O areas with a percent difference > 10%
Standard was not run	No runs associated with this standard were identified

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 is commented out. If ever the 9.52 standard is fixed, uncomment all “Comment 1” comments



function defined in gc_functions.R

function defined in gc_helper_functions.R