

Creation of output spreadsheets

Start with sample results

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

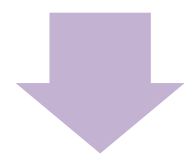


Get the N₂O calibrants

- 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 N₂O area and calculate the mean
- Determine the mean N₂O area for each calibrant



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



Assign flags to N₂O calibrants (see Flags)



Fit linear models using the N₂O 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)



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

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 N₂O values using the linear models

- Use the 0.98 model’s N₂O values when the N₂O values <= 1
- Otherwise, use the 80 model’s N₂O values



Store one output spreadsheet for each input spreadsheet

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

Calibrants are:

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

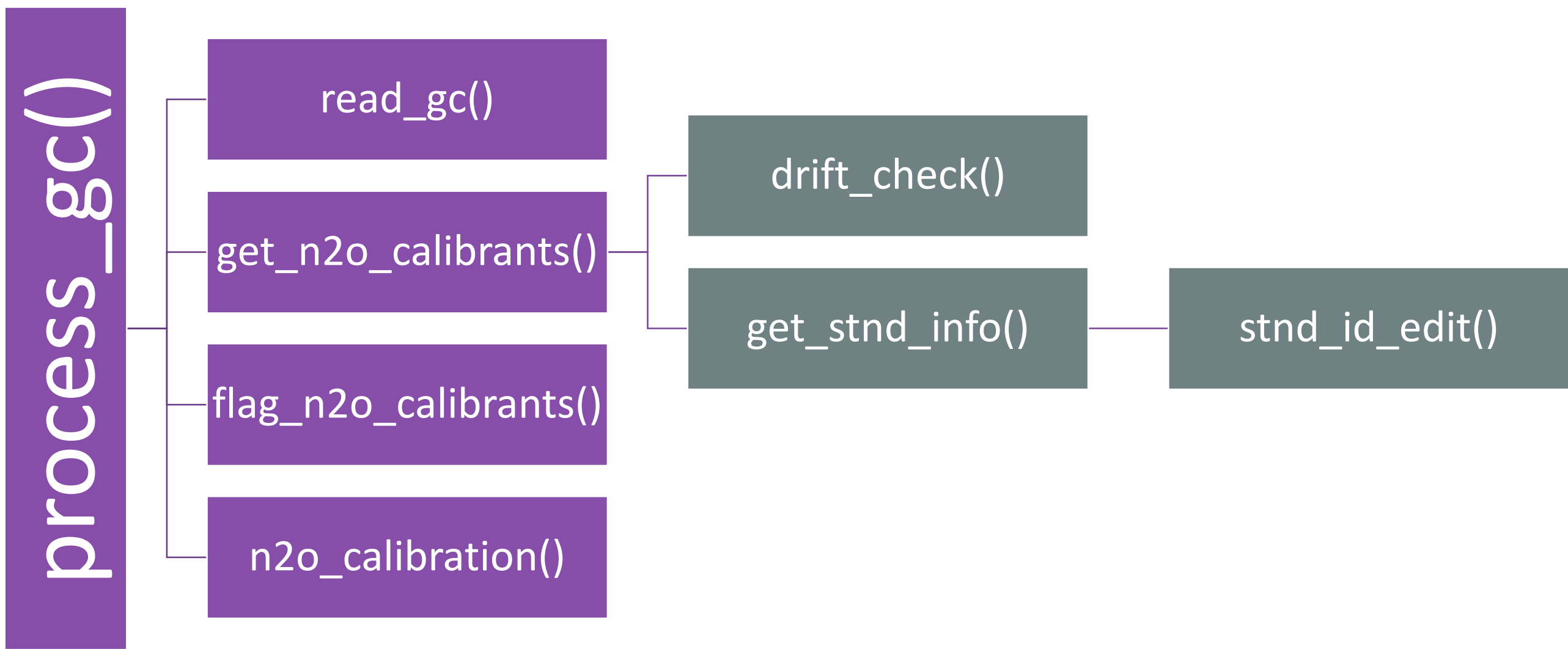
Flags

Flags for N₂O standards

Flag	Meaning
All areas are zero	All runs associated with this standard returns a 0 N ₂ O area
One non-zero area	Only one run associated with this standard returns a non-zero N ₂ O area
Low N ₂ O reproducibility (percent difference: #)	When standard returns two permissible N ₂ O 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