

# 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 N<sub>2</sub>O 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<sub>2</sub>O area and calculate the mean
- Determine the mean N<sub>2</sub>O area for each calibrant



Assign flags to N<sub>2</sub>O calibrants (see Flags)



Fit linear models using the N<sub>2</sub>O 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)



Calculate N<sub>2</sub>O values using the linear models

- Use the 0.98 model’s N<sub>2</sub>O values when the N<sub>2</sub>O values <= 1
- Otherwise, use the 80 model’s N<sub>2</sub>O values



Adjust recorded values to account for dry air instrument standards



Store one output spreadsheet for each input spreadsheet

Script functions on the premise that input files’ 1<sup>st</sup> sheet contains the data.

Calibrants are:

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

If you identify strange behaviour in the standards flags, check if some IDs could be mistaken for calibrants (they contain the numbers or strings listed above).



Used to identify which standards are associated with “High” IDs but do not contain the associated ppm amount in their name



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

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



$$\text{adjusted values} = (\text{measured values}/10^6) * (1 - p_{H_2O}/101.325) * 10^6$$

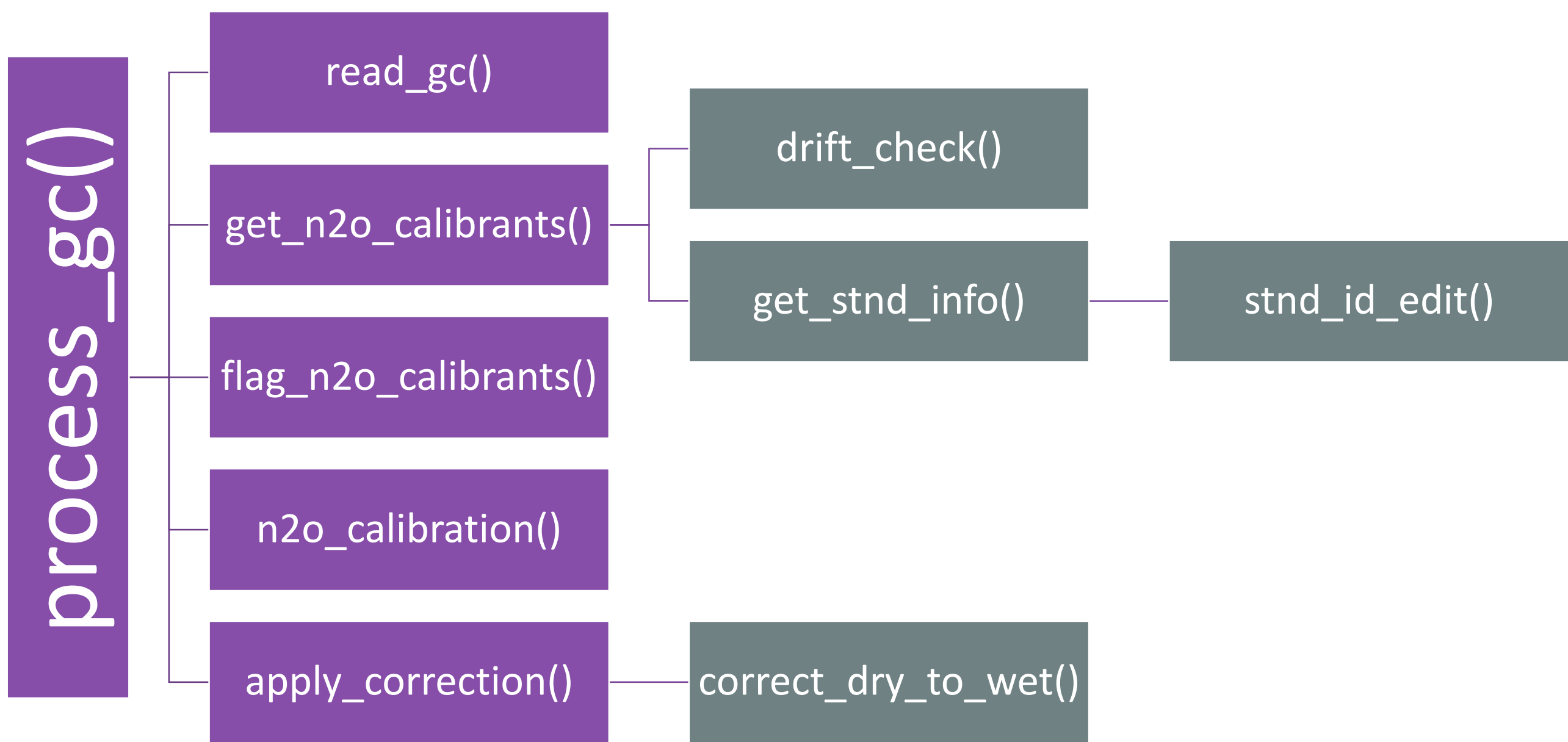
# Flags

## Flags for N<sub>2</sub>O standards

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