Flux Calculation

These files are associated with and produced by the authors of "Natural Geologic Methane Emissions from Microseepage in the Michigan Basin are Negligible" by Kathleen R. Hall, Thomas Weber, Marika Stock, Marc Buursink, Haoran Piao, Mingzhe Zhu, Katey Walter Anthony, Vasilii Petrenko (currently in review) and should be credited as such. More details on the methods related to these scripts can be found there.

The scripts in this set can allow for quick data visualization, processing, and flux calculation from flux chamber measurements. This includes allowing the user to interactively select measurement time windows and filter data, to generate and save figures of gas concentrations, to account for chamber volume and area adjustments, and calculate fluxes.

These scripts are meant to be used to calculate the flux from flux chamber measurements which use an online, continuous gas analyzer (e.g. a portable CRDS or LGR UGGA). This approach uses a "multi-slope method" wherein the slope of the gas of interest is calculated in 1-minute increments stepping every 10 seconds. These slopes are averaged, and the standard error is taken to arrive at a slope and error that is representative of the measurement and yields an accurate uncertainty which can be used to calculate the flux. For example, measurements with large disturbances to the chamber will have higher uncertainties.

Example concentration data, auxiliary data ("FieldNotes.xlsx"), and chamber dimensions ("Chamber_Area_Volume.xlsx") from the dataset of fluxes in "Natural Geologic Methane Emissions from Microseepage in the Michigan Basin are Negligible" is available in the folders.

How to use the scripts:

1. Replace the chamber dimensions and auxiliary data (e.g. chamber/air pressure and temperature) in the excel files "Chamber_Area_Volume.xlsx" and "FieldNotes.xlsx" with your data. Rename the sheets according to the names of your instruments and chambers which should match the input to the variables "instrument" and "chamber_type" on lines 14 and 15 of the main script.
2. Place your instrument data files into the "data" folder and change the "foldername" variable in the main flux calculation script, "FluxCalculation.m". The dataset should be inputed as a timetable called "ConcentrationData". In lines 26-54, change the variable for the gas concentration to the appropriate one from your instrument data.
3. Change the gases measured for each instrument to match your instrument (line 27 and 41). Also change the molar mass values and units to match the gases measured for each instrument.
4. Adjust any uncertainties associated with your measurements (e.g. pressure uncertainty, temperature uncertainty, etc.) before line 84 where the for loop begins.
5. Adjust the "date" and "sample" variables to the measurements you would like to run. Then run the script.
6. When Figure 1 pops up click where you would like to select the start time for your measurement, hit "Enter", then repeat again for the stop time.

7. Input in the command window when prompted whether you would like to filter the data ("Y") or not ("N").
    a. If you input "Y", it will ask for a window to filter. This is the number of data points to the right and left of where you will manually select which will be filtered out. The higher the number, the larger the portion of data that will be removed. Then, you can click on the figure which points to filter out and hit enter (similar to step 6).
    b. A message in the command window will ask if you are finished filtering. Respond "N" to select more points to filter out or respond "Y" to finish filtering.
    c. Tip: use large variations in cavity pressure to decide what data points to filter out.
    d. If more than 30 seconds of data is removed, you will be prompted to refilter. This 30 second limit can be adjusted on line 83.
8. Another figure will pop up on the screen with the concentration data plotted and the calculated flux. You will be asked whether "this flux makes sense" in the command window.
    a. If you respond "N", the current plot will be saved in the folder titled "ProblemSamples_Figures" for later inspection and potential recalculation.
9. This will repeat for all the selected samples or all the samples on that date (depending on your inputs at step 5).
10. After running all the samples, a results table will pop up on the screen will the flux calculations, uncertainty, and different parameters to be able to rerun the script.

Note: Small variations between fluxes calculated from the provided data may be slightly different to the published data set due to very small (less than a second) differences in the times selected for the start and stop of the measurements and small adjustments to uncertainties for specific samples.