Standard Operating Procedure
Infrared Gas Analyzer (IRGA) CO_2 measurement by integration method

Brief description:

This method uses continuous measurements (every second) from the Infrared Gas Analyzer (IRGA) unit to measure the CO_2 concentration of a gas sample. The method described here only details the use of a python script to convert the raw continuous data into discrete sample-by-sample integrations. The output is an excel spreadsheet with each sample's integrated CO_2 value and the time at which it was taken. This output can then be copied into your sample spreadsheet.

Materials:

A spreadsheet must be created during the gas sampling that notes the time that each sample was pushed through the IRGA. Excel has a timestamp function that you can automate with a 'Macro' to output the date and time down to the second at the press of an assigned keystroke.

Procedure:

Create a spreadsheet where you mark the samples with the timestamp that corresponds to the time when the gas sample was taken and injected into the IRGA.

Open the IRGA software on the lab computer and create a new file in a designated folder (this is important for the next steps) by clicking on the red 'record' circle. **Make sure that your filename has no spaces (ex. '5_20_20_data.txt' not '5/20/20 data.txt').** Note the 'background' CO_2 level when just N_2 gas is flowing through the IRGA. This is the threshold for splitting samples that you will input into the script. Keep track as this concentration may fluctuate during sampling. You can 'Zero' the IRGA after the background CO_2 reading stabilizes. If the baseline during sampling is 0.0 ppm CO_2, and your injections are correctly spaced (no overlapping output), then a threshold of 1.0 ppm CO_2 will work fine.

Begin injecting samples, marking their timestamp on your spreadsheet. Only inject the next sample after the CO_2 reading is consistently below the chosen threshold. Once all samples have been injected, click the 'stop' icon on the IRGA software and shut down the software.

Open the folder that you just created with the IRGA output file in it and drag the python script titled 'IRGA_Raw_data_processing.py' into that folder. This file will be located online with a website called Github for you to download a copy of. Go to this address to retrieve the file:

https://github.com/grantfalvo/Robertson_Lab_SOP_scripts

Then search for and open the program called 'Spyder (Anaconda3)' (see Figure 1 and 2 below). Then click 'File – Open' and open the file in your newly created folder titled

'IRGA_Raw_data_processing.py' (Figure 3). The code should populate one of the panels in the program (Figure 4). You do not have to write or even read any of this code. Do not change any of the code in the original file as this is a common file for everyone's use. If you would like to make your own changes please create a copy separate from the original file.

To run the script click 'Run – Configuration per file' (Figure 5). You must do this each time you run the script in order to enter the proper arguments. Next a window with the Run Options will appear (Figure 6). Leave the defaults but select the box called 'Command line options' and type the following into the text box next to this option:

filename.txt 1.0 1.0

where file name is the name of your raw IRGA output file followed by the extension '.txt' (remember that there can be no spaces in your filename), and the first '1.0' is your threshold value discussed above in ppm of CO_2 (defaults to 1.0 ppm CO2). This value can be changed to what is best for your sampling run. The second '1.0' value is the frequency of measurements that the IRGA is running at (defaults to 1.0 seconds). After this is filled out click 'Run' in the Run Options window and the script will run in a few seconds (some trivial errors will appear even during successful runs). A new Excel file will be automatically created in the folder that you just created with the same filename as the raw IRGA output file but with the '.xlsx' extension.

This is your output file and should have the following structure:

group	**area**	**Time(H:M:S)**
0	103.693	19:02:53
42	409.471	19:03:54
64	919.701	19:04:38
91	1605.24	19:05:31

Where:

there are 3 columns for group, area, and time
groups are random ascending numbers (not important what the numbers are)
areas are large positive numbers (this is your data)
time is an ascending clock times corresponding to when you sampled (this is when you sampled according to the lab computer clock)

You can then copy these 'areas' into your spreadsheet with the timestamps. If your spreadsheet has each sample entered in the same order that you sampled, then you can just copy and paste directly because the python script outputs the samples in the order that they were injected into the IRGA.

This is a highly flexible script if you know how to use python (please do not modify the original on the lab computer). Any questions can be directed to Grant Falvo (908-917-2770).

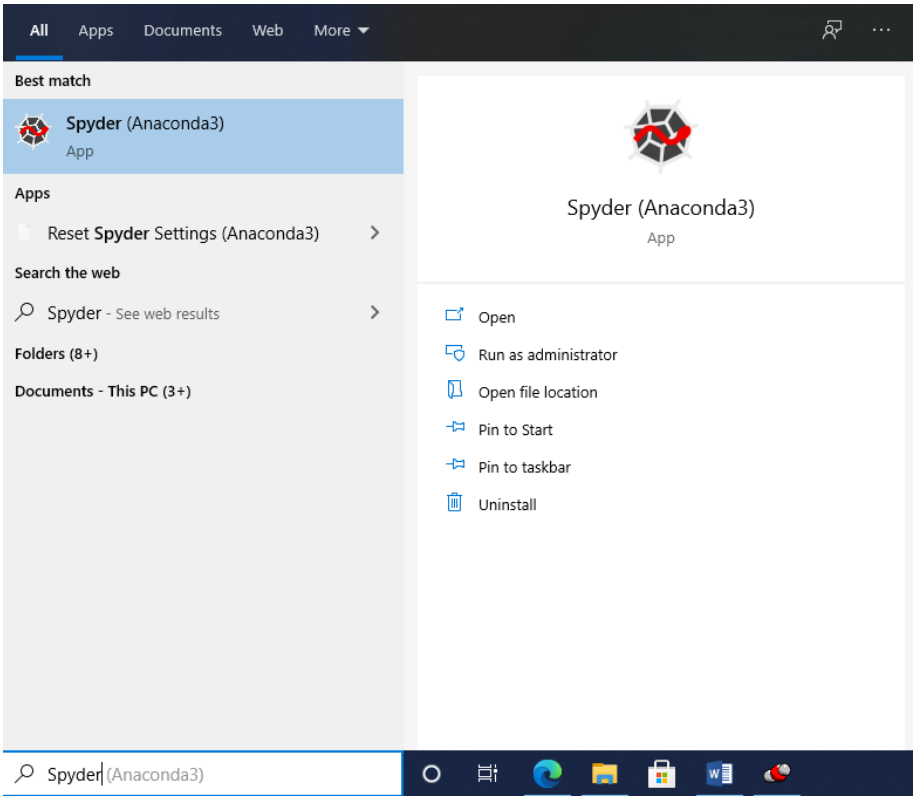

Figure 1.

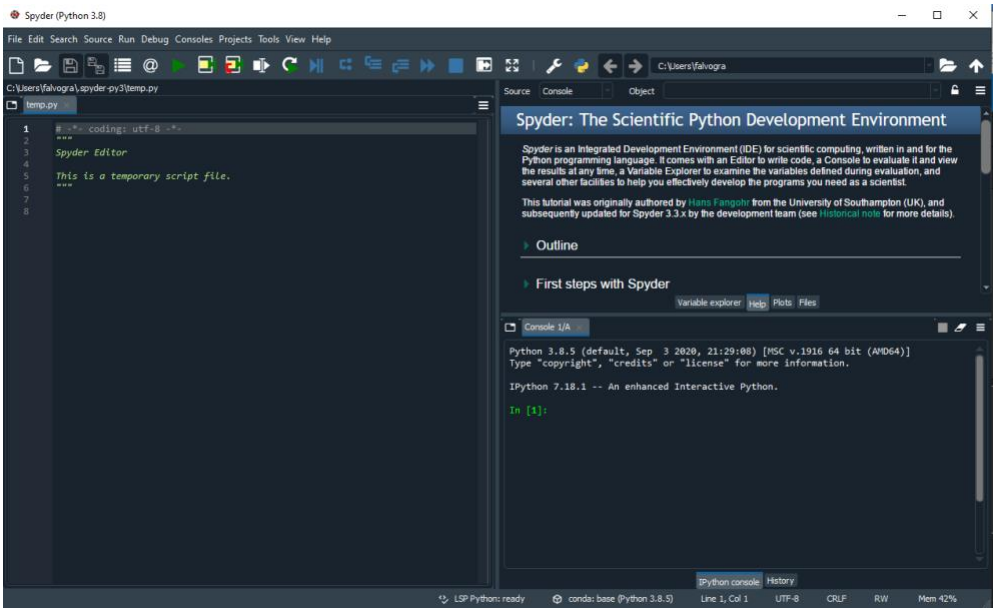

Figure 2.

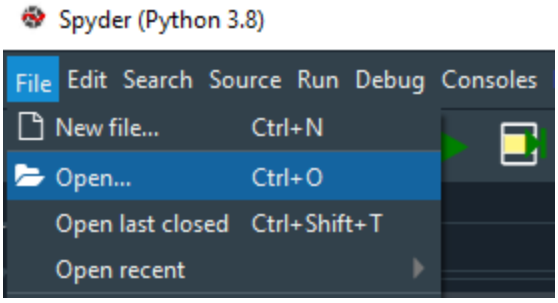

Figure 3.

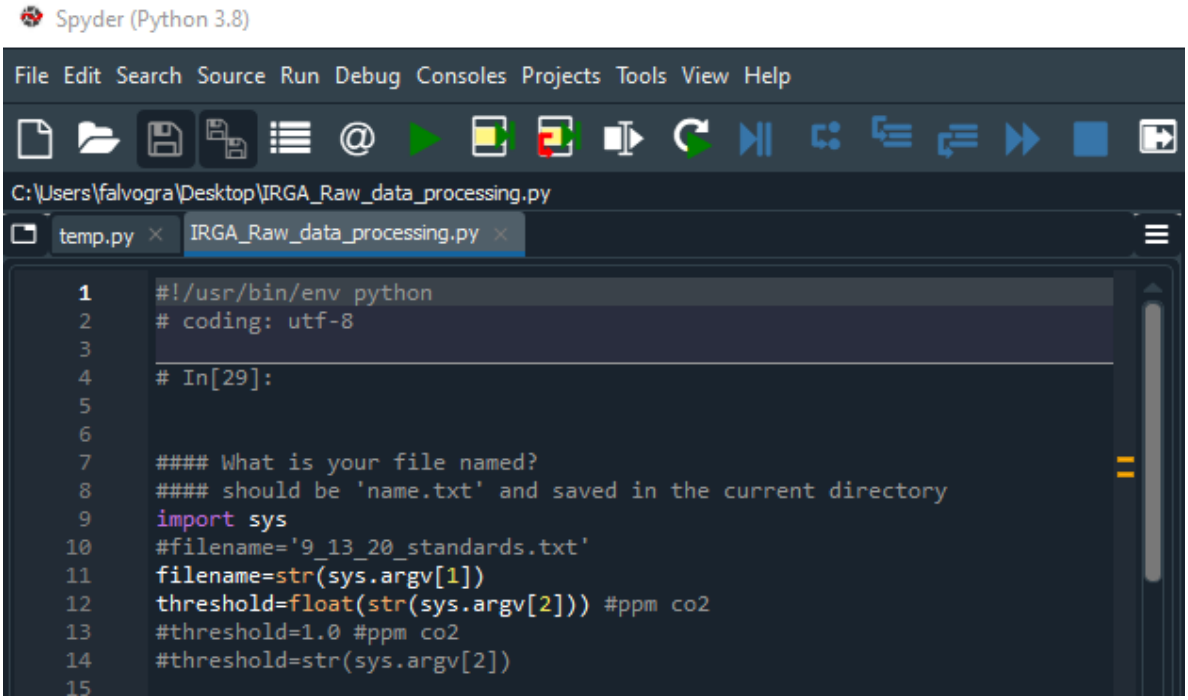

Figure 4

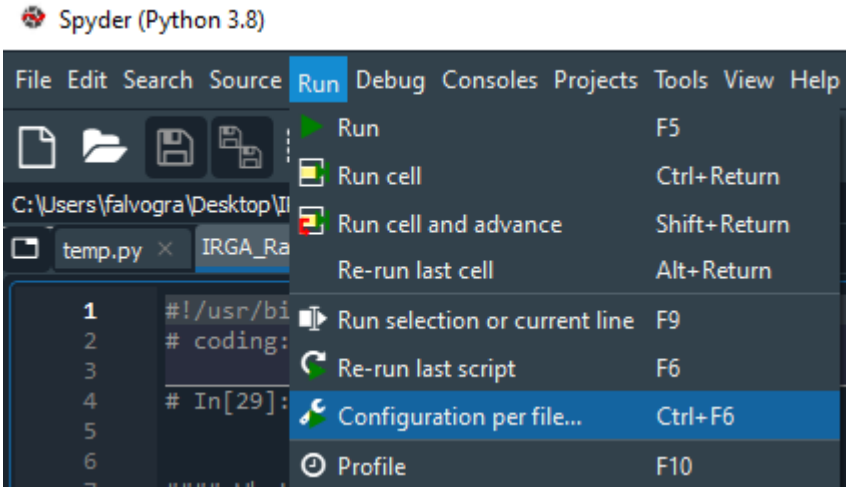

Figure 5

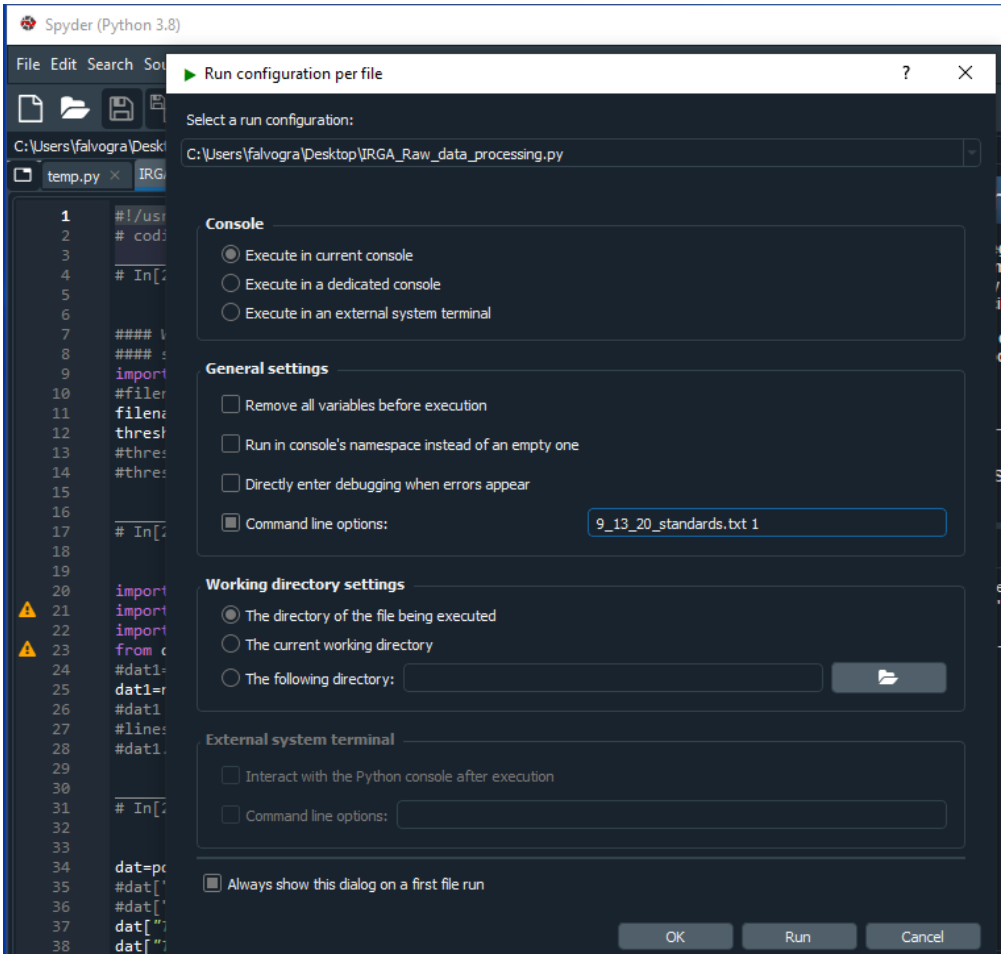

Figure 6

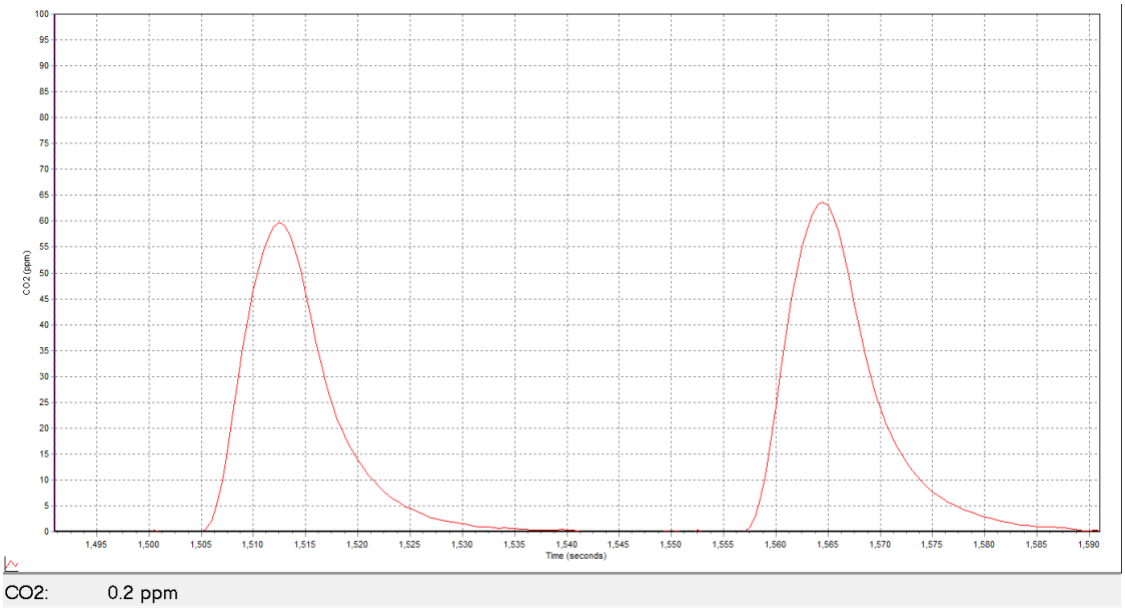

Figure 7