Mass Spectrometer Refinement

Processing eight points of voltage data

Cousins Photosynthesis Lab in the School of Biological Sciences at WSU

Team WM Codeworks

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I. Introduction

Our team has been tasked with creating the fifth module for the mass spectrometer used by the Washinton state university's photosynthesis lab for the school of biological sciences. The spectrometer we will be working with measures the different species of gases in a sample. This is useful for classifying gases and running biological experiments with them. Previous teams have created a visual interface and methods for inputting data from a mass spectrometer with python code. These other four modules are related to a mass spectrometer with three points of measurement; Our task will be pertaining to a machine with eight points of measurement. The collected data will be used to visualize and make calculations with the composition of the gas being analyzed in the machine.

II. Background and Related Work

A mass spectrometer is a device which can be used to identify unknown compounds and also to measure the quantity of known compounds. This is done by exploiting the weight of ionized particles and their interaction with strong magnetic fields. A mass spectrometer does this in the context of this project by accelerating a gas mixture around an electromagnetic. As the molecules cycle around the magnetic field, they are distributed into a spectrum based off weight. Lighter molecules move more dramatically than heavier molecules. For example, CO2 at 32 g/mol is affected less by the field than O2 at 32 g/mol. Inside the chamber which contains the cycling gases is an array of voltage detectors. These detectors are calibrated to be positioned in the zones of known molecules. Larger quantities of a specific gas give a stronger reading on the detector and vice versa. This, in conjunction with the proper software, allows the operator to learn about the specific molecular make up of a gaseous mixture as well as its proportion. The results of this tool allow researchers at WSU, specifically in the photosynthesis lab, to run experiments on the effects of different gas mixtures on plant behavior, as seen in Ellsworth *et al.* [1]. In summary, mass spectrometers yield highly accurate compositional information, establishing the critical foundation upon which many scientific experiments are built. Previous teams working on this project created software modules which take input from the spectrometers and provide visuals and tools to make calculations on specific user defined parameters. The spectrometer in this case utilized three detectors. Our team will be responsible for creating similar software modules with specific client needs for another spectrometer which utilizes an array of eight different detectors. This allows for the identification different and measurement of different gases and additionally measurement of different species of molecular isotopes. This will be useful for experiments since different molecular isotopes or isotopologues behave differently in various plant processes. Our team will need to get familiar with how the spectrometer handles output. Pre-existing code should cover most of that particular process, but it may be required for working with the other machine. In addition to this requirement, our team must have an acceptable proficiency in working with the programming language Python, as all previous code has been written with it and uses specific python libraries. Preexisting software exists to allow the output of the spectrometers to be visualized StellarNet [2]. However, the client is requesting specific Python modules to be developed for specific experiments and for the sake of maintainability and future development.

III. Project Overview

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The goal of this project is to develop a data acquisition, manipulation and presentation software for the Photosynthesis lab. More specifically they require a software application that can record live data from a mass spectrometer and plot that data live to a graphical user interface. Users

should be able to record calibration measurement off the live data and specified timepoints in the record data. We are the 4th team to work on this project, with previous teams already bringing the software to state where it has basic functionality that meets all of the initial requirements. The overarching goal in our team's development on this project are to improve functionality of the existing 4 modules and develop a module 5 that combines data from three distinct instruments that records and plots the data in a similar manner to modules 1 2 and 3.

IV. Client and Stakeholder Identification and Preferences

Our primary client is WSUs Photosynthesis Lab. The lab is primarily managed by Dr. Asaph Cousins, who is the primary point of contact between our team and the lab. We are working closely with him to ascertain the preferences and needs of him and his team and ensure that we are improving the project in the manner which is most beneficial to him and his team.

The primary stakeholders of this project are Dr. Asaph Cousins and the graduate students and postdoctoral researchers who work in the lab. The needs and preferences of these stakeholders is for the already existing measurement to be improved to be more powerful allowing it to perform additional functions. Additionally, the software must be modified to allow it to take measurements from additional scientific instruments. These stakeholders also require all changes and additions made to the software to be heavily documented; allow them or additional teams they hire to work and make changes to the project.

Additional Stakeholders include WSU and other researchers who benefit from discoveries in the relevant fields that the Photosynthesis Lab works on. As the photosynthesis lab is owned by WSU, improvements to the speed and effectiveness of the lab's research help make the lab more valuable to them. Other research in the relevant fields of study will also benefit from the improved efficiency of the research output from the Photosynthesis Lab caused by the improvements to our project.

V. Glossary

Mass Spectrometer: A device that detects the presence and abundance of specific molecules.

Isotope: A variant of an atom or molecule which differs in weight.

Electromagnet: A device which can be used with electricity to create and tune a magnetic field.

VI. References

[1] P. Z. Ellsworth, M. J. Feldman, I. Baxter, and A. B. Cousins, “A genetic link between leaf carbon isotope composition and whole-plant water use efficiency in the C_4 grass *Setaria*,” *Plant Journal*, vol. 102, no. 6, pp. 1234-1248, Jun. 2020. doi: 10.1111/tpj.14696.

[2] StellarNet Inc. “SpectraWiz LabVIEW Software.” StellarNet.us. Accessed: Sept. 12, 2025. [Online]. Available: https://www.stellarnet.us/software/spectrawiz-labview-software/