Mass Spectrometer Interface

A Desktop Application for Reading Instrument Data

Cousins Photosynthesis Lab in the School of Biological Sciences at WSU



**Team Linnaea Borealis**

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Kyler Kupp, Erik Holtrop

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# Introduction

When plants breathe, they take carbon dioxide (CO2) out of the air and replace it with oxygen (O2). Determining what affects plants’ respiration rate, or their breathing rate, is incredibly valuable data. These factors point backwards in time, reflecting causes for evolutionary trends, and forwards in time, providing opportunities to improve agriculture. We can use a mass spectrometer to measure this breathing rate. The mass spectrometer measures the amount of CO2 and O2 in the air, and so the respiration rate is the change in each of those.

The Cousins Photosynthesis Lab in the School of Biological Sciences at Washington State University uses one of these mass spectrometers. These instruments are complicated devices, requiring complex calculations for calibration. The lab uses proprietary software from the mass spectrometer’s manufacturer, but that software outputs massive amounts of data over the course of a multi-hour lab, most of which isn’t needed. This problem has been partially solved with the creation of a Python desktop application, but this application is not perfect. Our task is to improve this application. This application currently faces small bugs, and only works for one instrument. The application is also in process of a UI upgrade. There’s also a few non-spectrometer instruments in the lab that are provide similar data, that would be easier to use if their data-streams were combined.

# System Requirements Specification

## Use Cases



**Calculate Bicarbonate/CO2 Ratio**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Compute the ratio of bicarbonate to carbon dioxide using specific selections of mass spectrometer data. |
| Pre-conditions: | * File path to folder containing CSV files including bicarbonate and carbon dioxide data has been selected. * Bicarbonate and CO2 have both been calibrated by selecting at least 2 segments of data per molecule where they are present in different concentrations. |
| Related Requirements | * Calculate Ratio * Center Mean Bars |

**Plot Derivatives**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Accurately plot the ratio of CO2 49 to all present molecules on one graph and plot its derivative on a second graph. |
| Pre-conditions: | * File path to folder containing CSV files including bicarbonate and carbon dioxide data has been selected. * Bicarbonate and CO2 have both been calibrated by selecting at least 2 segments of data per molecule where they are present in different concentrations. |
| Related Requirements | * Plot Derivatives |

**Convert Data**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Convert the data from new mass spectrometer so that it matches the format of data output by the original mass spectrometer. This will allow the data to be used by the existing programs in modules one, two, and three. |
| Pre-conditions: | * Data is actively being output from the mass spectrometer’s proprietary software. |
| Related Requirements | * Format Data |

**Select Input Files**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Select input files for data from three separate instruments. The instruments being used are as follows: LI-COR Leaf-gas Exchange System, tunable diode laser (TDL), and Picarro (measures different oxygen isotopes). |
| Pre-conditions: | * All three instruments are outputting a stream of data. * Data inputs are correctly formatted. |
| Related Requirements | * Ability to Seclect Data Streams |

**View Graph**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | View three streams of data being plotted to a graph in order to analyze the exchange between CO2 and water in leaves. |
| Pre-conditions: | * Input file locations have been selected |
| Related Requirements | * Plot Data Streams |

**Manipulate Graph Scale**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Manipulate the scale of the graph in the application. |
| Pre-conditions: | None |
| Related Requirements | * Ability to Manipulate Scale |

**Change Plotting Speed**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Manipulate the scale of the graph in the application. |
| Pre-conditions: | * Input file locations have been selected * Data stream has not yet run out of data |
| Related Requirements | * Ability to Change Plotting Speed |

**Select Data Points**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Select two data points using mean bars so that a smaller portion of data can be analyzed. |
| Pre-conditions: | * Input file locations have been selected * Data has been plotted to graph |
| Related Requirements | * Mean Bars |

**Calculate Mean**

|  |  |
| --- | --- |
| Actors: | Lab researcher |
| Goal: | Calculate the mean value between the two mean bars (selected data points). |
| Pre-conditions: | * Input file locations have been selected * Data has been plotted to graph * Mean bars have been arranged in desired position |
| Related Requirements | * Calculate Mean Values |

## Functional Requirements

### Calculating Concentrations (Module 1)

**Calculate Ratio:** The application must feature a button that allows the user to calculate the ratio of bicarbonate to carbon dioxide. This button will display the ratio in decimal format.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to record the ratio for use in their research.

**Priority**: Priority Level 0: Essential and required functionality

**Center Mean Bars:** The application must visually present mean bars in the center of the graph window. These bars can be moved and used to calculate the mean of a selection of data.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to prevent the means bars from spawning off-screen and causing confusion or requiring additional effort.

**Priority**: Priority Level 1: Essential and required functionality

### Analyzing Enzyme Activity (Module 3)

**Plot Derivatives:** The application must provide the ability to plot the ratio of carbon dioxide with mass of 49 units to all present molecules. Additionally, the app must be able to plot the derivative of the ratio graph.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to analyze the exchange of oxygen and monitor the rate of enzyme activity.

**Priority**: Priority Level 0: Essential and required functionality

### Data Conversion (Module 4)

**Format Data:** The application must convert data from a new mass spectrometer into a specific format so that it can be analyzed using existing applications. The data must be converted from hexadecimal to decimal format and split into small CSV files.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to increase the speed of their research by incorporating a second mass spectrometer.

**Priority**: Priority Level 0: Essential and required functionality

### Analyzing Exchanges in Leaves (Module 5)

**Ability to Seclect Data Streams:** The application must be able to select file sources to pull from for data from three different instruments. These instruments include a LI-COR Leaf-gas Exchange System, a tunable diode laser (TDL), and a Picarro that measures different oxygen isotopes.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need to be able to analyze data from all three instruments to get a fill picture of the exchange between carbon dioxide and water in leaves.

**Priority**: Priority Level 1: Desirable functionality

**Plot Data Streams:** The application must plot each of the three data streams on a graph. The graph must be able to plot data dynamically in near-real time.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to analyze the exchange between carbon dioxide and water in leaves.

**Priority**: Priority Level 1: Desirable functionality

**Ability to Manipulate Scale:** The application must provide the ability to manipulate the scale of the graphs. The user should be able to edit the lower and upper bound of both the horizontal and vertical axis.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to get a satisfactory view of the graph so that trends can be observed.

**Priority**: Priority Level 1: Desirable functionality

**Ability to Change Plotting Speed:** The application must provide the ability to change the speed at which the data is plotted as well as pause the plotting of data.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to conveniently plot data at a speed that allows for easy observation.

**Priority**: Priority Level 1: Desirable functionality

**Mean Bars:** Two vertical bars must be included in the graph of the application. The user should be able to move the bars to encapsulate a desired segment of data from which the mean can be calculated.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to accurately and quickly record the mean of specific segments of data.

**Priority**: Priority Level 1: Desirable functionality

**Calculate Mean Values:** The application must provide the ability to calculate the mean value between the two mean bars.

**Source**: The client at the Cousins Photosynthesis Lab originated this requirement. The client and lab researchers need this feature to accurately and quickly record the mean of specific segments of data.

**Priority**: Priority Level 1: Desirable functionality

## Non-Functional Requirements

Our project exists in the context of academic plant biology research, and thus has several ideals and values it strives to represent and uphold. These ideals don’t necessarily describe what the program *does*, they rather describe how it *is*. This section clarifies the non-functional requirements which we’ll use to guide our design and development to uphold these ideals and values.

**Modern Visuals:**

The system shall look like a modern 2020’s program. PyQt5’s baseline UI elements meets this standard

**Python For Extendibility:**

The system shall use Python since it is one of the most common languages among Biology students, including those that use the Cousins Photosynthesis Lab. This will enable extension and maintenance.

**Documentation For Extendibility:**

The system shall have documentation for code that’s thorough enough to allow college senior skill level software engineers to extend and maintain it.

**Documentation For Non-Technical Users:**

The system shall have documentation to enable non-technical users to make full use of it. For example, an explanation of how to create executables of each module.

**Accuracy:**

The system shall accurately calculate and portray data. The instruments have their own levels of accuracy, so maintenance of significant figures should be enough.

**Compatibility:**

The system shall use the established data format, which is versatile enough to work with other devices.

**Non-Destructive:**

The system shall not overwrite or otherwise destroy any data.

# System Evolution

The Cousins Lab’s relationship with WSU places it in a position to enlist Computer Science students to work on this codebase each year as part of their capstone. We see this in the project’s history, having two teams as previous maintainers. The sponsor liaison, Dr. Cousins, has voiced an intention to have software created for many of the instruments in the lab. With these considerations, we should make our software compatible with different machines if possible, and make it maintainable and extendable by software engineers with the skill and education level of a college senior.

We can see what this looks like from the issues and opportunities presented by previous teams. For instance, the modules written from the lab’s primary Mass Spectrometer, may be usable for the second one, provided we write software to reformat its data stream. In another case, some of the existing code lacks basic files to enable maintenance, like a requirements.txt for relevant Python libraries or the context files for executable creation.

# Glossary

**Mass spectrometer:** an apparatus for separating isotopes, molecules, and molecular fragments according to mass. The sample is vaporized and ionized, and the ions are accelerated in an electric field and deflected by a magnetic field into a curved trajectory that gives a distinctive mass spectrum.

**UI**: User Interface. The means by which the user and application interact.

# References