SENIOR DESIGN 2 Water Contaminant Analysis through Raman Spectroscopy



Department of Electrical Engineering and Computer Science University of Central Florida

Dr. Lei Wei

Academic Committee: Dr. Peter Delfyett, Dr. Murat Yuksel, Dr. Matthieu Baudelet

Sponsor: Ocean Insight

Group 5 CREOL

Julia Smith-Blanchard: Photonic Science and Engineering George McDonald: Photonic Science and Engineering Juan Restrepo Diaz: Electrical Engineering Gibran Khalil: Electrical Engineering Sebastien Jouhaud: Computer Engineering

Table of Contents	Table	e of	Cor	ntents
-------------------	-------	------	-----	--------

1.0 Executive Summary1	
2.0 Project Narrative2	
2.2 Background3	
2.3 Project Description3	
2.4 Project Goals and Objectives3	1
2.5 Similar Projects5	I.
2.6 Requirement Specifications6	
2.7 House of Quality Diagram7	
2.8 Project Milestones8	
2.9 Project Budget and Financing9	
2.10 Block Diagrams	. 10
2.10.1 Optical Visual Diagram	. 11
2.10.2 Software Block Diagram	. 14
3.0 Related Research16	
3.1 Existing similar technologies16	
3.2 Relevant Technologies – Raman Spectroscopy and the SHS21	
3.2.2 Humidity and Temperature	. 24
3.2.3 Safety Systems	. 25
3.3 Wired communication protocols26	
3.4 Strategic Components and Part Selection	
3.4.1 Spatial Heterodyne Spectrometer Components	. 31
3.4.2 Raman Illumination System Components	. 35
3.4.3 Temperature & Humidity Sensor Components	. 37
3.4.3.1 SHT33-DIS-B2.5kS	. 37
3.4.3.2 SHT40-AD1F-R2	. 38
3.4.3.3 HIH6030-021-001	. 38
3.4.4 Computer Options	. 40
3.4.4.1 Processor	. 41
3.4.4.2 RAM	. 43

3.4.4.3 Storage	44
3.4.4.3 Operating System	46
3.4.4.4 Computer Selection	48
3.4.5 Microcontroller Options	49
3.4.5.1 MSP430FR6989	50
3.4.5.2 MSP430G2553	51
3.4.5.3 STM32G431C6T6	51
3.4.6 Power Supply Options	. 52
3.4.7 XY table	. 55
3.4.7.1 MOXY-01-100-100	55
3.4.7.4 Comparison Table of XY-Tables	. 57
3.4.8 Voltage Regulators	57
3.4.8.1 MAX25302BATD/V+	59
3.4.8.2 LM317MDT-TR	60
3.4.8.3 TPS563300DRLR	61
3.4.9 Pad Shaping & Sizing	64
4.3 Optical Components	
4.3.1 Diffraction Gratings	
4.3.2 Lenses)
4.3.2.1 Intaging Lens	
4.3.4 Fiber Collimator	,
4.4 MATLAB Calculations	
4.5 Spectrometer Design in ZEMAX	
4.6 – Prototype Spectrometer	
4.7 – Well-plate reader and Illumination System	
4.8 Sample Usage	
4.8.1 Sulfur	
4.8.2 Ammonium Nitrate	97
4.8.3 Potassium Perchlorate	
4.8.4 Sodium Sulfate	101
5.1 Design Standards	108

5.1.1 Power Supply Standards	
5.1.2 IEEE 802.3 Standards	
5.1.3 IPC PCB Standards	110
5.1.4 RoHS Compliance	
5.1.5 Laser Safety Standards 5.1.5.1 Class 1 Lasers 5.1.5.2 Class 1M Laser 5.1.5.3 Class 2 and 2M Lasers 5.1.5.4 Class 3R and 3B Lasers 5.1.5.5 Class 4 Lasers	111 112 112 112 112 112 112
5.1.6 Electrical Safety Standards	
5.2 Design Constraints	115
5.2.1 Economic and Time Constraints	116
5.2.1.1 Economic	116
5.2.1.2 Time constraints	116
5.2.2 Environmental, Social, and Political Constraints	117
5.2.2.1 Environmental	117
5.2.2.2 Social	117
5.2.2.3 Political	117
5.2.3 Ethical, Health and Safety Constraints	118
5.2.3.1 Ethical	118
5.2.3.2 Health and Safety	120
5.2.4 Manufacturability and Sustainability Constraints	121
5.2.4.1 Manufacturability	122
5.2.4.2 Sustainability	122
6.0 Project Hardware and Software Design Details	125
6.1 Initial Design Architectures	126
6.2 First Subsystem	130
6.3 Second Subsystem	131
6.4 Software Design	133
6.4.1 Supplemental Software	141
6.4.2 PCB Design Software	143

6.4.2.1 Altium	
6.4.2.2 EAGLE	
6.5 Summary of Design	
7.0 Administrative Content	
7.1 Bill of Materials	
7.2 Finance	
7.3 Team Organization	
Appendix A: References	

1.0 Executive Summary

As pollution becomes an ever more present problem in our society, people often wonder how their food and drinking water will be affected by these chemicals, pesticides, and contaminants that have become so prevalent in the way things are made. Pesticides cover our grasses and run off into our aquifers, air pollution is absorbed into the rain and falls back down into the oceans and wells. Acid rain is a serious threat to Floridians due to the daily afternoon thunderstorms that we experience. Coupled with the train derailments in Ohio that poisoned the area, the average person is bound to be worried about their overall health faced with all the health hazards that invade our means of life. For that reason, we have decided to develop a Raman spectrometer that will be able to detect the contamination levels of any liquid sample.

As pollution becomes an ever more present problem in our society, people often wonder how their food and drinking water will be affected by these chemicals, pesticides, and contaminants that have become so prevalent.

The goal of this project is to create a Raman spectroscopy platform for identification and measurement of pollutants that is common in water. The focus of this project will be identifying contaminants such as heavy metals and organic pollutants. The system will be created to be user-friendly and can be applied to other fields not only the applications related to water.

The team created a specifically designed Raman spectroscopy system that featured a 532 nm laser, a fiber optic probe, and a spectrometer to accomplish this objective. The performance of the system was tested using a variety of actual water samples obtained from diverse sources after it had been calibrated using a set of standard samples with known contaminant.

The finding that we want to show is that the system was able to identify and measure a variety of contaminants, such as sulfur (etc..) samples. The system is suitable for a variety of applications in environmental monitoring and water quality testing since it can identify toxins at different levels of the environment and where people are at the most.

2.0 Project Narrative

The overall quality of our drinking water is vital to the health and well-being of all living species on planet Earth, including humans. But as residents of the state of Florida, we are constantly reminded that not all water is good to drink. Between the ocean that surrounds our peninsula and the springs, aquifers, retention ponds, lakes, and rivers within Florida, water is a large part of our day-to-day existence.

Due to all the different sources of water, knowing which ones are safe to drink is essential to avoiding any kind of infections from water contaminants. Furthermore, sometimes even our drinking water isn't safe to drink (for example, the leadcontamination water crisis in Flint, Michigan). Additionally, it is common for herbicides from lawn care or contaminants from retention ponds to leak into our rivers and underground wells. Thankfully, the EPA works hard to ban chemicals like DDT from being used to prevent our water from tainting our water sources and our water utility companies have filters and methods to remove these contaminants from our water. However, these methods of removing pollutants can only be so effective and sometimes the methods end up adding things that are just as harmful. It is a commonly known fact that our drinking water either has naturally occurring fluoride in it or has added fluoride "to help reduce the incidence of cavities among the population." On the contrary, 98% of western European countries have banned the practice of fluoridation for various reasons. The most concerning of said reasons is that the "chemical used to fluoridate water is an industrial waste product from the phosphate fertilizer industry. It is an unprocessed hazardous waste, contaminated with several toxins, particularly arsenic."

The goal behind our project is to create a portable water quality analyzer using Raman spectroscopy. We believe that being able to determine what contaminants are in our water should be public knowledge and allows the people to be able to have a say in what is in our water. Moreover, if we can test any source of water anywhere in the state then inhabitants of an area can quickly become aware of any impurities, which would reduce the number of water-related illnesses. By using Raman spectroscopy, we can use lasers with a preset wavelength along with sensors calibrated to those wavelengths to be able to detect a predetermined set of contaminants. The reason for the preset wavelengths and contaminants we are detecting is because each contaminant is detected only at a certain wavelength, so our lasers and sensors must be calibrated to detect things appearing in that specific range. The advantage of this type of analysis is that Raman spectroscopy returns very accurate results at a fast rate.

The water spectrometer will come with features that will be user friendly. Several key functions that will be included are detection of different contaminants that are present, a software application toolkit for data analysis and dual sensing. Our project will be sponsored so we must abide by their requirements. They have asked us to build a small version of a spectrometer that will work and fit into their

well plate reader. The spectrometer configuration that we have use is interferometric, a spatial heterodyne spectrometer. This spectrometer will be connected to a fiber that collects light scattered from a variety of samples illuminated by a laser of certain output wavelengths. This information will be processed and sent to a computer where spectral information will be presented on an GUI.

2.2 Background

The senior design experiment will feature how to use a spectrometer to analyze water. The type of spectrometer that will try to be implemented in the design is a spatial heterodyne spectrometer (SHS). The SHS offers great resolution and through a compact design. It functions by splitting the incoming light into multiple beams using a beam splitter and reflecting the first order diffracted light back into the splitter, where they then interfere with each other and produce a string of fridge. The spectral information is encoded in this interference pattern, or interferogram. By taking the Fourier transform of this "barcode" interferogram, the spectral information would then be shown through a CCD camera and analyzed through some external display. The spectrometer will be able to detect at least 1 or different contaminants in water. The aim is to have bacteria and metals that could be harmful for consumption to be detected in this design.

2.3 Project Description

A spectrometer and its illumination system are important tools to help give knowledge that could not be acquired either way. It is a method of understanding molecules and how they interact with light. By analyzing the amount of light absorbed or emitted through a sample we can determine the characteristics of the sample.

2.4 Project Goals and Objectives

The goal of this project is to build a portable, cost-effective Raman spectrometer that focuses on mainly measuring the contaminants in different water samples. We aim to *measure at least 2 different contaminants*. Objectives are good to have to make sure that you are having standards for your project and that it is being fulfilled the prototype will meet the following goals:

Cost - The device will cost less to build than models that are currently in the market while it is performing the same task. The funding part of the project will be mostly covered by our sponsor, Ocean Insight, since they are giving us some of the equipment that we need.

Size - The size of the device will be portable and not too bulky. The idea of the size was set because of the constraints. The spectrometer must be able to fit inside a well plate reader for water analysis.

Ease of Use - The device will be simple and not overly designed. Many wires and other external accessories will not be needed for this project. Also, the device will have access to a smartphone to be able to process results.

Utility Analysis - The device will be able to give classification of the water analysis. Should be able to detect which contaminants are in the water and the percentages.

Quality – The device will have to be handled carefully to ensure that the optical or electrical components are not ruined.

The **core goals** of this project are to identify the presence of contaminants in samples of natural and publicly used water instantly. Also, to develop a system that is easy and accessible for a user to operate. Lastly, perform measurements on two different samples in a way that is non-destructive.

The **advanced goal** is to produce a setup that is modular to provide more options for users. While doing this it will identify and separate several different contaminants, both with pre-defined amounts of water safely.

The **stretch goals** are to solidly identify with no ambiguity what contaminants is present in a pre-treated natural water sample. Also, while converting the spectrum to a text that tells you what the contaminant is that you are will be scanning. Finally, provide percentages of contaminants.

The projective goals listed above will be met by the end of senior design 2. The core goals are the main goals must be met by the specifications what we put on the project. The advanced and the stretch goals will be implanted in the project if we can get working in a timely manner.

The objective of this project goes hand and hand with meeting the goals. The **core objectives** of this project are to develop a compact spectrometer that contains simple mounted optics. This would reduce spectral errors due to misalignment. Use Raman spectroscopy to perform noninvasive analysis of the samples. Lastly, to determine a suitable laser wavelength that will work across samples, most likely a laser wavelength of 532 nm.

The **advanced objectives** use a combination of a well-plate reader and a detachable spectrometer to achieve a modular set-up. We have been using a 532 nm wavelength and reduce fluoresce from signal. Then use an electro-mechanical device that allows the user to switch between samples easily and quickly without removing them or having to adjust optics. Lastly, to develop a PCB that can process that spectral data quickly.

Once we have fully completed our project it is important to have goals to achieve given that we have more time to complete it. These **stretch goals** are important because they allow us to increase the functionality of our system, make it more convenient to use, and allow us to be more creative when designing our system.

Our first stretch goal is to incorporate a computer into the system. Instead of having the user ensure that their computer can run MATLAB, having the program to connect to the system on hand, installing all the additional software required, and having enough ports to make all the connections, it would be significantly easier to have a computer built into the system. To do this, we would have to find a small, single-board computer with a screen attached. The Latte Panda brand of computers discussed in section 3.4.4.4 - Computer Selection would be a good choice to go with as they are relatively inexpensive, perform all the necessary operations to run the software, and some of their models meet all the system hardware requirements for our system.

A similar computer-oriented stretch goal would be to turn the various USB and ethernet connections into a series of wireless connections. This would most easily be done through either Bluetooth or a Wi-Fi connection with the module located within the system. However, this would still require the user to bring their own computer that can run the program, but the hardware requirements needed to make all the connections between the various components and the user's computer would be removed. Some of our other stretch goals are to produce a processing toll that can distinguish the different spectral components. Also, another objective we may pursue is to construct a spectral library that the software can reference.

These are the goal and requirements that we have come up with as a team on all parts of our team. In senior design 1 going on senior design 2 we have tried to get to our goals and objectives one by one. We have made sure that everything works well and is up to our standards. These advanced goals and objectives if not completed in senior design 2 at least our core goals will be completed.

2.5 Similar Projects

<u>Raman Spectroscopy for In-Line Water Quality Monitoring — Instrumentation and</u> <u>Potential</u> – This paper is less about the applications of Raman spectroscopy but more about the general background information of what is Raman spectroscopy and how the instruments for it are evolving day after day. It also discusses possible uses for the equipment that is being developed.

<u>Applications of Raman Spectroscopy in Detection of Water Quality</u> – This project focuses on the various applications of Raman spectroscopy for detecting

contaminants in water are presented based on the various types of pollutants that may occur. These include organic and inorganic as well as any biological contaminants. The project also discusses any limitations to be using Raman spectroscopy for this sort of application. These limits include detection materials, limits of detection, detection range, peak positions, and selectivity. It finishes the paper by going over how Raman spectroscopy can be used in future water quality analysis projects.

2.6 Requirement Specifications

Design constraints and requirements are an important topic to be discussed. This section will consider things we have need to be able to succeed in our senior design project. This part needs to be specific in what we want to the project to make sure that we are not too flexible about we want. The constraints in this project will include not only cost but what the sponsor's idea for what the project outline is supposed to be. The specifications are important to the sponsor because they will use this product in the future.

Specifications		
Samples to measure(<i>at least two)</i>	Potassium Perchlorate, Ammonium Nitrate, Sodium Sulfate	
Spectral range	532 nm to 618 nm	
Hardware Control	GUI fully operates well-plate motor and laser	
Computation of Raman Spectra	Software performs image processing of Fizeau fringes	
Integration time	≤ 10 seconds	
Wavelength	532 nm	
Sample size	40 ml	
Laser power	≥ 50 mW	
Spectrometer dimension	3.5" x 2.5" x 1.2"	
Raman spectrum resolution	$\leq 20 \ cm^{-1}$	
Safety interlock engagement time	Instantaneously	

From the above requirements, we have chosen the three demonstrable requirements to be used for the end of the semester demonstration. If anything needs to be adjusted, it will be reflected in this table.

The three requirements in the specification table that are highlighted as stated before will be having to be demonstrated in the final demonstration at the end of the semester. However, all the requirements will try to be completed by the team.

2.7 House of Quality Diagram

The engineering house of quality diagram shows the trade-off matrix for the spectrometer. It was designed to show the difference between its engineering and marketing requirements. An explanation of what the house of quality diagram is showing will be shown. The engineering requirements list is shown from the perspective of the developers of the product. Product dimensions describe the volumetric size of the SHS. This shows that the product will be a portable device in theory. The number of components will show the cost effectiveness compared to other devices that are already out on the market.



2.8 Project Milestones

These are the project milestones that were created to keep the team diligent and motivated. These project milestones will be for both semesters through senior design 1 and 2.

Week	Milestone	<u>Dates</u> (SD1 & SD2)	<u>Status</u>
1	Brainstorming	January 9 - 13	Done
2	Project Selection	January 16	Done
3	Divide and conquer	February 3	Done
4	Research and Building Optical Theory	February 2	Done
5	Writing Paper	February 8-10	Done
6	Senior Design 1 Draft	Feb 13	Done
7	Finalizing Paper	March 24	Done
8	Final Document	April 25	Done
9	Conceptual Prototype	April 25	Done
10	Start Building Application	June 15	Done
11	Design and Order PCB	June15	Done
12	Get PCB and Optical Components Together	June 30	Done
13	Design and Build Enclosure	July 1	Done
14	Final Testing and Revisions	July 27	Done
15	Final Presentation	END	

2.9 Project Budget and Financing

Our project will not be self -funded and will instead be funded by our sponsor, Ocean Insight. The individual parts will be given or funded to us by the company. The total cost can be calculated from the below estimates of cost for each component except for having no malfunctions. Ocean Insight will also be providing all necessary test equipment and lab space during the product testing phase. The final product design produced will be used as a prototype for what they wish to use in the future.

ITEM	QUANTITY	PRICE ESTIMATE
Laser	1	Sponsored
Gratings	2	~\$160
Lens	3-4	~\$260
CCD	1	\$700
Motor translation stage	1	Sponsored
Well plate reader with additional components	1	Sponsored
Polarized beam splitter	1	\$880
Power Source	1	\$10
Custom PCB	1-2	\$80
Custom Enclosure	1	\$50
Microcontroller	1	\$15
Connectors	3	\$10
Misc. Components	TBD	\$30
TOTAL	N/A	~\$2160

2.10 Block Diagrams

The block diagram below shows the division of responsibilities and overall schematic of the spatial heterodyne spectrometer. The device starts with a power supply that will turn on the illumination system and a motor control for the samples. The laser that will be used will excite the samples so that both metal and bacteria metal will be shown when analyzing. The laser will then be passed into the optics area of the device where the optics will separate the spectrum and pass it to the sensor array.



2.10.1 Optical Visual Diagram

Pictured below are the 3D models of the sampling case containing several cuvettes where the samples are to be placed as well as a conceptual drawing of the spatial heterodyne spectrometer and its fundamental components. A fiber would collect the light scattered from the sample inside of the cuvette and carry that signal to the SHS. Once the laser is focused on the samples it will be illuminated. The light that we expect to see would be the Raman signal. This will then be imaged upon the detector. The way the SHS operates will be described in further detail.



Well plate reader - contains illumination system and spectrometer

Figure 3 - Optical block diagram for spectrometer



Figure 4 - 3D impression of well plate containing cuvettes.

A three-dimensional picture is shown above of the cuvettes. The model is an inaccurate model because the cuvette is not that tall. The cuvette stops at the top part of the metal horizontal place keeping it together.

Cuvettes are important for tools in analytical chemistry because they are used to hold and contain small volumes of liquid samples for spectroscopy in our case. They are multiple reasons why cuvettes are important. Cuvettes allow for accurate measurement of liquid samples by containing them in a small volume with a known path. Cuvettes come in various shapes, sized and material to accommodate for different types of analysis. They can also be standardized, meaning that their dimension and properties that are optically driven are well-defined and consistent, this allows for more accurate and reliable measurements, as well as easier comparison results between different labs or experiments. Cuvettes can also be used for quality control purposes to ensure the accuracy and precision of measurements.

The decision of whether to use circular or square cuvettes may be influenced by the needs and preferences of the experiment. Because they offer more sample surface area for excitation and detection, square cuvettes can have certain benefits for fluorescence experiments. Because they provide a more uniform route length and reduce the influence of light scattering, circular cuvettes may be preferable for absorbance measurements. The final cuvette shape will be determined by the application and experimental conditions. Cuvettes in the project with Raman spectroscopy is important as all the reasons above. But with Raman spectroscopy additional precautions need to be considered. In Raman spectroscopy, it is important to use a small volume to reduce risk of photobleaching of the sample. Samples are sensitive, therefore cuvettes with a small volume are typically preferred. The Raman signal strength and overall sensitivity of the measurement can be impacted by the sample's transit through the cuvette. Although longer paths might produce a louder signal, they might also make photodegradation more likely. It is crucial to select cuvettes with a route length that is suitable for the sample and measurement circumstances.

The Raman signal strength and overall measurement sensitivity may be impacted by the sample's journey length through the cuvette. Stronger signals may be obtained from longer paths, but photodegradation risk may also rise. Because of this, it's critical to select cuvettes with path lengths suited for the sample and measurement circumstances.

Raman spectroscopy cuvettes should be built of a substance that is transparent in the desired spectral region (usually in the visible or near-infrared range) and does not contribute to the Raman signal. For cuvettes in Raman spectroscopy, common materials include quartz, glass, and plastic.

The choice between circular and square cuvettes in Raman spectroscopy may be influenced by the needs and preferences of the experiment. Circular cuvettes are typically favored because they reduce light scattering and offer a more consistent route length. For some applications, however, where a greater sample volume or a longer route length are sought, square cuvettes may be helpful. In the end, the requirements should determine the cuvette shape.



Figure 5 - General 3D representation of the SHS

Pictured above are the 3D models of the sampling case containing several cuvettes where the samples are to be placed as well as a conceptual drawing of the spatial heterodyne spectrometer and its fundamental components. A fiber would collect the light scattered from the sample inside of the cuvette and carry that signal to the SHS. The way the SHS operates will be described in further detail. In the prototype that we have be creating soon. The optical team will be starting the first steps of the spectrometer. The design will allow for a smaller and more compact instrument without compromising the spectral resolution.

To guarantee an even split of the input light and precise alignment and overlap of the two beams, the beam splitter must also be carefully constructed. To further minimize the instrument's size for a prototype with 1/2-inch lenses, a smaller beam splitter might be utilized, also of ½ inch size. The performance of the instrument will also be impacted by the optical component architecture. Smaller optical parts might be employed in a SHS prototype with 1/2-inch optics to reduce the size of the device. To ensure appropriate functioning, the components must still be carefully positioned.



Figure 6 – SHS visualization

2.10.2 Software Block Diagram

The block diagram below demonstrates how the code interacts with each other and depends on certain steps to be completed before other actions can be performed and features can be accessed. The initialization of the motor, laser, and spectrometer must first occur before any settings of those components can be edited. Once those have been set to the user's specifications, the user may move on to the separate run tab that has a variety of options to run the spectrometer and analyze the desired well as necessary.



3.0 Related Research

In this section of our report, we have described the related technologies and sciences that inspired the project as well as its design. Although this project is an exercise in engineering, it is still important to discuss the relevant concepts of Raman spectroscopy as well as other spectroscopy types, the union of optical and electrical engineering to construct a spectrometer, and other existing technologies and products that inspires our design to simplify the task of measuring contaminant levels in water.

3.1 Existing similar technologies

The steps involved in detecting and treating water can vary depending on the source of the water and the type of contaminants present. However, in general, the process involves the following: water sampling, analysis and detection, treatment, quality control, and distribution.

Once an appropriate detection tool is realized, samples are selected from the desired source. Levels of contaminants of a variety of types may be detected and depending on that contaminant type, treatment may or may not be considered and the treatment method is selected. According to the CDC, water treatment can be generalized in the following manner: coagulation, flocculation, sedimentation, filtration, followed by disinfection. (Prevention, 2022)

The focus of this project and our design is to develop a tool that is reasonably priced and capable as much as other technologies to determine the type of contaminant and potentially the level of that contaminant within our samples of water. We would like to demonstrate that the use of Raman spectroscopy through a configuration of a spatial heterodyne spectrometer can do this task. But first, let's consider other available technologies that are on the market now.

Gas chromatography mass spectroscopy, or GC-MS in short, is a sensitive technology that can separate large volumes of water samples from low to high concentrations of all kinds of contaminants such as VOCs, pesticides, and industrial chemicals. Volatile organic compounds come from cosmetics, room deodorizers, fabric, paint, fuels, and adhesives. (Moran, 1986-99) Pesticides can come from synthesized chemical substances designed to control pests ranging from insects to weed and fungi. GC-MS is a technology that can separate the individual components of the mixture of water and contaminants. It uses gas chromatography where a sample is injected into a column that contains a gas.

This mixture is then separated based on physical and chemical properties like molecular weight or boiling point. These separated components are then carried through the column and into the mass spectrometer where they are ionized by electron impact ionization for detection and analysis. The mass spectrometer then provides a spectrum, or a fingerprint of the ionized components. (McMaster, 1998)

The first step is to separate the individual components of the mixture using gas chromatography. In this step, the sample is injected into a column that contains a stationary phase and a carrier gas is passed through the column. The components in the mixture separate based on their physical and chemical properties, such as boiling point, polarity, and molecular weight. The separated components are then carried through the column and into the mass spectrometer.

Injection Source



Figure *8* - Simple diagram illustrating GC-MS.

Some models of this approach can be small, and benchtop sized, while others can be quite large depending on the application and environment in which this approach is used as well as the desired accuracy and sensitivity of the results. If it isn't clear, this approach can be quite complex, however accurate. GC-MS uses a gas chromatograph, and a mass spectrometer which itself consists of an ionization source, mass analyzer and a detector. The gas chromatograph itself can cost about \$30,000-\$50,000. (How Much Does A Gas Chromatograph Cost?, 2022) The price of a mass spectrometer from a simple search online can range from \$10,000 to well over \$100,000. So not only is GC-MS complex and time consuming, but it is also quite expensive. But it is certainly not a bad approach as it can be quite accurate and provide excellent results.

Having discussed concepts using a variety of unintroduced terms, it is appropriate to briefly describe spectroscopy in general. Spectroscopy is a scientific technique that allows us to analyze the composition of a substance by looking at how it interacts with light. Every substance interacts with light in a unique way, and by analyzing the light that is absorbed, emitted, or scattered by a substance, we can learn about its chemical composition and structure. In the case of our project, one can determine the presence of contaminants by analyzing the spectrum of a sample.

Ultraviolet and visual light absorption by contaminants can be used to identify them. (Spangenberg, 2021) The fundamental principle here is that ultraviolet light is

shined on a sample of some substance, some of this light is absorbed and some is emitted. What scientists would measure is the amount of light that the sample absorbs. Different substances absorb UV and VIS light differently, depending on their chemical composition. For example, pollutants, pigments, or natural organic matter can absorb UV light at specific wavelengths. A device that could be capable of this is a spectrophotometer, which is a device that has some light source contained within it as well as a spectrometer. The details of the latter will be further elaborated upon in future sections.

The light from a spectrophotometer is shined upon a substance, some of the light is absorbed and some is emitted. This light is often collected by fiber and carried to the spectrometer. The spectrometer can be composed of a variety of optical components in different configurations. The spectrometer configuration can be selected based on application and desired results as well as a variety of other factors. Regardless, the ultimate measurement of such a device as a spectrophotometer is an absorption spectrum, with the y-axis representing the intensity of light that reaches the detector inside, vs. an x-axis representing the wavelength of light. See the figure on the next page for an example. There is also infrared spectroscopy, which uses the infrared portion of the electromagnetic spectrum to analyze samples.



Though UV-VIS spectroscopy is an extremely well-known and popularly used technique, one of its main limitations compared to, for example, Raman spectroscopy is its lack of specificity. While UV-Vi's spectroscopy can provide information about the overall absorbance or transmission of a sample at certain wavelengths, it cannot differentiate between different types of chemical groups or

specific molecular structures in a complex mixture. The spectra of substances can sometimes be unique, but there are cases where the spectra can overlap or blur. In the case of water contaminants where the sample could potentially contain a variety of substances, the likelihood in which the spectra doesn't fully capture all the information would increase.

In contrast, Raman spectroscopy can provide more detailed information about the chemical bonds and molecular structure of a sample, allowing for more specific identification of contaminants. Raman spectroscopy works by measuring the inelastic scattering of light, which can provide information about the vibrational modes of chemical bonds in a sample. This allows Raman spectroscopy to distinguish between different chemical groups and molecular structures.

As mentioned previously, there are a variety of spectrometer configurations, each that have their own pros and cons. One example of a configuration is the Czerny-Turner. The Czerny-Turner configuration can suffer from low throughput due to the multiple optical elements in the system, including the entrance and exit slits, collimating and focusing mirrors or lenses, and diffraction grating. This can result in a loss of light intensity and reduced sensitivity. Stray light can also be a problem in the Czerny-Turner configuration due to the presence of multiple optical elements and the potential for reflections and scattering. Stray light can reduce the accuracy and precision of the measurement and can be difficult to eliminate completely.



Figure 10 - Czerny-Turner Configuration

Another potential issue in this configuration is thermal drift. If the spectrometer is not temperature stabilized, changes in temperature can cause the position and angle of the optical elements to change, which can affect the accuracy and precision of the measurement. Other configurations of spectrometers include the Littrow configuration and the Ebert-Fastie configuration. The Littrow configuration can achieve high resolution and uses fewer components than other configurations. It can be quite compact and is simple in design. This configuration consists of a light source, a plane diffraction grating, and a spherical collimating mirror. The diffracted order of interest is then reflected to an exit slit.



Figure 11 - Littrow configuration

However, like the Czerny-turner, this configuration can be privy to wavelength drifts caused by temperature changes or mechanical vibrations. Any changes in the angle of the grating can affect the position of the diffracted light. It may also have limited throughput, since the collimating mirror and focusing mirror must be positioned very precisely to achieve optimal performance.

The Ebert-Fastie configuration has the light source and the entrance slit placed at one side of the instrument, and the detector on the other. It can also be compact and provide a wide wavelength range for use. Similarly, to other configurations however, limitations due include mechanical stability limitations as well as complex light paths.



Figure 12 - Ebert-Fastie config

Though these issues can be nitpicky, it only heightens the case for the use of another configuration of particular interest, the Spatial Heterodyne Spectrometer (SHS) which will be further described in detail in the following of this report.

3.2 Relevant Technologies – Raman Spectroscopy and the SHS

To grasp what our group is attempting to accomplish, we have dive into a concise explanation of Raman Spectroscopy as well as the Spatial Heterodyne Spectrometer. This is a new type of device that was introduced in the 21st century.

Raman spectroscopy can be a very powerful tool for identifying molecules and substances because it provides a unique fingerprint of their chemical composition. When a sample is illuminated with a laser beam, the scattered light contains information about the chemical bonds and vibrations present in the sample. This information is unique to each substance and can be used to identify even very complex molecules.

One of the great advantages of Raman spectroscopy is its ability to identify substances even in complex mixtures. Since each substance has a unique Raman spectrum, it is possible to isolate and identify individual components within a mixture, even at low concentrations. This makes Raman spectroscopy a valuable tool for a wide range of applications, from forensic analysis and drug discovery to environmental monitoring and materials science. The basic idea behind Raman spectroscopy is that when a sample is illuminated with a laser beam, some of the light is absorbed by the sample, while some of it is scattered in different directions. Most of the scattered light has the same frequency as the incident laser beam, but a small fraction of it has a different frequency. This frequency difference is called the Raman shift. Raman spectroscopy aims to identify a substance by taking advantage of the vibrations and rotations of molecules by measuring the scattering of light.



Figure 13 - Principals of Raman Scattering

The scattered light in Raman spectroscopy has a different frequency and energy than the incident laser beam, which provides information about the chemical composition of the sample. When the scattered light is collected and analyzed, it reveals the unique Raman spectrum of the sample. This spectrum provides a unique "fingerprint" of the chemical bonds and vibrations present in the sample, which can be used to identify the substance.



Figure 14 - Example of Raman spectrum of water

There are two main types of scattering that can occur in Raman spectroscopy: Rayleigh scattering and Raman scattering. When a molecule absorbs energy from the incident laser beam in Raman spectroscopy, it begins to vibrate and rotate in various ways. These vibrations and rotations are specific to each molecule, depending on its chemical structure and composition. As the molecule vibrates and rotates, it may interact with the surrounding electrons and atoms, causing small changes in the electronic and vibrational energy levels.

When the molecule emits this energy as scattered light, it can do so in one of two ways: Rayleigh scattering or Raman scattering. In Rayleigh scattering, the scattered light has the same energy and frequency as the incident laser beam because there is no exchange of energy between the molecule and the photon. In Raman scattering on the other hand, the scattered light has a slightly different energy and frequency than the incident laser beam because some of the absorbed energy is transferred to the molecular vibrations and rotations.

This energy transfer leads to the unique Raman spectrum of the sample, which is essentially a "fingerprint" of the chemical composition of the sample. Each peak in the Raman spectrum corresponds to a specific vibrational or rotational mode of the

molecule, and the intensity and position of the peak provide information about the strength and symmetry of the chemical bonds in the molecule. For the purposes of this report for Senior Design, we won't dive too deeply into Stokes and anti-Stokes Raman scattering. Our approach in our engineering will rely on the support of experts that surround us as well as comparison to known Raman spectra.

Next, we have described the Spatial Heterodyne Spectrometer (SHS) and make a case for why this is an appropriate configuration for our attempt in designing a Raman system for the analysis of contaminants present in water.

The SHS is unique compared to the previously mentioned configurations. The SHS has applications ranging from astronomy, atmospheric science to environmental monitoring. This device can have a high throughput, which makes it attractive for astronomy purposes. It can also measure very slight changes in wavelength, meaning it can achieve high resolution.

The components that construct this device include two diffraction gratings, a beam splitter, focusing and imaging optics, and the detector. The setup is like the Michelson interferometer, which is an interferometric optical device that measures differences in the length of two paths of light. This device, like the SHS consists of a beam splitter, but replace the gratings with two mirrors. The light splits at the beam splitter, each beam reflects off the mirrors and recombines at the splitter where it is guided to the imaging arm. Depending on the difference optical path lengths between the two beams, constructive or destructive interference of the reflected light from the moveable mirror with the light reflected from the fixed mirror can occur, producing intensity fringes at the imaging plane.

Replace the mirrors in the Michelson interferometer with diffraction gratings at equal distances from the beam splitter and you have an SHS, an interferometric spectrometer.



Figure 15 – Michelson interferometer diagram

The SHS is attractive due to its potential high resolution, increased sensitivity, high throughput, increased spectral range, lack of need for scanning with no moveable parts, propensity for compactness, as well as potential low cost. Though the result of this device is an interferogram (a pattern formed by the interference of two beams of light), this image can be Fourier transformed and converted into a conventional spectrum with intensity vs. wavelength. This device can potentially be very useful in Raman spectroscopy as broad spectral ranges and high throughput are valuable in attaining the weak Raman signals that are used to identify our contaminants in water.



Figure 16 – Schematic of Spatial Heterodyne Spectrometer

The details of this device as well as the mathematics will be elaborated upon in the parts selection as well as the optical design description later in this report. However, it should be noted that the focus of this report is less about the SHS itself and more on the engineering of an SHS for use with Raman spectroscopy for the purposes of analyzing contaminants in water for our senior design project.

3.2.2 Humidity and Temperature

Temperature and humidity are critical factors in the performance and accuracy of a spectrometer's measurements for various reasons. These environmental conditions have a direct impact on sample stability, instrument stability, and calibration, which ultimately determine the reliability of the analytical results. Hence it is a concept that should be highly controlled. These direct impacts are seen more deeply in functionality as:

In sample stability, fluctuations in temperature and humidity can lead to physical, chemical, or biological changes in the samples being analyzed. For example, temperature variations can affect the solubility, chemical equilibrium, and reaction rates of analytes in the sample, which could result in inaccurate measurements. Changes in humidity can also cause the evaporation or condensation of water in the sample, altering its composition and concentration. Therefore, uncontrolled temperature and humidity can lead to inconsistent results and compromise the reliability of the analysis.

As for the instruments used, spectrometers consist of highly sensitive optical and electronic components, such as light sources, detectors, and devices that can be influenced by environmental conditions. Temperature and humidity fluctuations can cause changes in the optical properties, alignment, and performance of these components, leading to drifts, signal intensity variations, and reduced accuracy. Uncontrolled environmental conditions can negatively impact instrument stability, causing unreliable measurements and the need for frequent recalibration and maintenance.

Accurate calibration of spectrometers is essential for precise and reliable measurements. Temperature and humidity can impact the calibration process by affecting the properties of calibration standards, the performance of the instrument's components, and the stability of the baseline. Failure to account for environmental variations during calibration can result in systematic errors in the measurements, undermining the validity of the analysis.

The fact that we are dealing with water quality and therefore, water samples, these factors play a huge role for the correct functionality of our project as we are aiming for accurate results as well as not having failures overall. We have explored this topic more when we immerse into the component selection as these factors will be sensed by devices that are going into the Printed Circuit Boards and in result, inside the spectrometer.

3.2.3 Safety Systems

Safety is extremely important for our project. The effects of lasers on human eyes have been extensively documented, and without any adequate safety systems implemented on our spectroscope, it will be very dangerous to operate. This can be seen by the power of the laser that we have be using, which is 150mW. As previously noted in previous sections, The first part of the safety system starts with the enclosure that will house our spectroscope. The enclosure will not allow lasers to escape the enclosure and cause damage to the people operating it. Naturally we must place our well plate with our samples into the enclosure to scan it. After placing the well plate, we have made sure that the enclosure will be completely

closed, and no lasers will be let out. A tinted window at the top of our enclosure will be used to close the spectroscope while in operation. After the window is closed, the well plate is locked in place. Once the locks are in place then we have started the timer, once this timer reaches its limit, the scanning process will begin. This timer is to make sure that the enclosure is securely locked and so that the operator cannot try to rapidly open and close the window to trick the safety interlocks. In the case that the safety interlocks are breached however, we have another safety feature in place. The second safety feature is a failsafe in case the first one fails. In case the window is breached during operation, it will cut off power to the laser, preventing any lasers from escaping the enclosure and ensuring safety of the operator. For the locking mechanism itself, an electronically actuated lock will be used, this will ensure that the lock will activate automatically, and takes away the option from the user to not lock it at all. For the power cut off feature, we have been using a relay that controls the power to the laser, this relay will be implemented on our breadboard.

3.3 Wired communication protocols

A key feature to keep in mind when selecting components is to look at the communication protocols that is needed to transfer data. In this section, we have introduced the concept of these technologies and how they are a huge factor in how our project works and how the different components both optical and electrical components that go in the PCB are able to communicate with each other and therefore realize the overall function of our senior design project. Wired communication protocols play a crucial role in ensuring the reliable and accurate transfer of data between various components, sensors, and devices. These protocols are essentially standardized sets of rules that govern how data is exchanged within a system.

In the search for communication protocols, we felt the need to only look at the ones we are familiar with. This would be serial communication technologies, which are the ones that transmits single bits of data from component to component at a time. This process is mostly done by a microcontroller that governs how this data is processed, sent, and received. Many of the components that we use in our project have their own communication protocol therefore learning about them is an essential task to ensure the proper functioning of our project. We have analyzed the different communication protocols to be seen in our project and how we have managed them using a microcontroller.

Signal levels, timing, data encoding, and the physical connections required for successful communication are some of the differences between the types of communication protocols. Protocol management ensures data integrity, synchronization, and error detection or correction, depending on the specific protocol being used by adhering to the specific rules of each one. Wired communication protocols, such as I2C, UART or SPI, cater to different

requirements and are chosen based on factors like speed, complexity, network topology, and application-specific demands, based on the requirements of the components at use.

<u>3.3.1 I2C</u>

The first communication protocol we have be introducing is I2C. Inter-Integrated Circuit is a two-wire, half-duplex, serial communication protocol. It uses a masterslave architecture where multiple devices can be connected in a bus topology only comprised by two wires as seen below in Figure XX. The two wires in I2C are the Serial Data Line (SDA) and the Serial Clock Line (SCL). SDA is used for data transmission, while SCL provides the clock signal to synchronize data transfer.

There is a clock signal coming from the master device through the SCL wire is one of the most important characteristics of the I2C communication protocol as the clock signal ensures that all devices on the bus are synchronized during data transfer. It coordinates when the data is sampled and when it is changed, thus preventing misinterpretation of the data being sent or received. The clock signal helps maintain data integrity by providing a clear reference for when data should be read or written. This ensures that the data is stable and valid at the time of sampling. In this way it also controls the speed at which data is processed within the system.



Figure 17 – I2C Wired Communication

Reprinted with permission from 911electronics from <u>https://911</u>electronic.com/how-i2c-works-i2c-protocol/i2c-connection-master-slave/.

I2C can support multiple masters and slaves. There is an addressing mechanism to identify individual devices on the bus in comparison to UART communication.

There is simple hardware implementation, requiring only two pull-up resistors. I2C is therefore suitable for applications and devices that may require lower data rates at relatively short distances. It is widely used for sensor interfacing, which is the main reason for the use of this protocol in our project.

<u>3.3.2 UART</u>

The second communication protocol used in this project is UART. (Universal Asynchronous Receiver/Transmitter) is a widely used serial communication protocol format wired by pin-to-pin that transmits data asynchronously, in contrast to I2C being synchronous.

The meaning behind this definition is that data transmission between two devices using UART does not rely on a shared clock signal to synchronize the communication. Instead, the sender and receiver devices operate independently with their own clock sources. In asynchronous communication, the data is transmitted in packets or frames, which consist of a start bit, some data bits, an optional parity bit for error checking, and one or more stop bits. The start bit and stop bits are used to indicate the beginning and end of a data frame, allowing the receiver device to synchronize itself with the incoming data being sent over.



Figure 18 – UART Wired Communication by Analog Devices

Reprinted with permission from Analog Devices from <u>https://www</u>.analog.com/en/analog-dialogue/articles/uart-a-hardware-communication-protocol.html.

UART employs separate lines for transmitting (TX) and receiving (RX) data as pictured in Figure XX these pins are the conditions for a successful wired communication in this protocol. UART communication does not require a clock signal, as it uses start and stop bits to synchronize data transfer between devices.

The absence of this shared clock signal makes UART communication simpler, and less hardware involvement compared to synchronous communication protocols. The biggest benefits of using a UART wired communication protocol are that simpler hardware and software implementation is a feature due to the asynchronous transmission with configurable baud rates. The fact there is no addressing mechanism, TX and RX pins wired up are all that is needed for two devices to communicate between each other.

In conclusion to these features, UART is commonly used in applications requiring simple, low-cost, and low-to-moderate-speed communication between two devices. Examples include Bluetooth modules, and microcontroller-to-PC communication this latter one, being the one we have use in our senior design project. UART communication will be used to connect the microcontroller in the PCB to the computer receiving all the data our project output and may need.

<u>3.3.3 SPI</u>

SPI, which means: Serial Peripheral Interface, is a synchronous serial communication protocol used primarily for communication between microcontrollers and various other components or sensors that support this protocol over a short distance. It is widely used in embedded systems and other electronic devices due to its simplicity, low cost, and ease of implementation. SPI is a full-duplex master-slave communication protocol which means that data can be transmitted and received at the same time between a master device and multiple salve devices interconnected.

This SPI protocol uses four signal lines which are represented in Figure 13 below: SCLK (Serial Clock): is generated by the master device to synchronize the data transfer between multiple devices connected.

MOSI (Master Out Slave In): is used for transmitting the data from the master device to the slave devices.

MISO (Master In-Slave Out): is used for transmitting the data from the slave device to the master device.

SS (Slave Select): is a dedicated line for each slave device which allows the master device to select which slave to communicate with by pulling the line low.



Figure 19 – SPI protocol by Corelis

Reprinted with permission from Corelis from <u>https://www</u>.corelis.com/education/tutorials/spi-tutorial/.

In SPI protocol the master device initializes communications by configuring the SPI interface such as polarity, bit data, and clock phase and then selects a slave device by pulling the SS line low and send a clock signal through SCLK line at a defined frequency. Data is then transmitted between the master and slave devices through the MOSI and MISO lines, with one data bit transferred per clock cycle. Once this data transfer is complete, the master device releases the SS line that was pulled low to begin the communication with the slave device at use, returning it to a high state, as the communication session ends between the master and slave devices.

SPI is to be used in situations where a reliable, and efficient communication protocol is needed for data exchange will between a microcontroller and connected component devices. It is suitable for applications with low data rates and short distances, such as communication with sensors, memory chips, displays, and ADC or DAC components.

3.4 Strategic Components and Part Selection

What we are ultimately building is a combination of a spectrometer as well as assembling a Raman illumination system. There will be a combination of a variety of optical components and devices, as well as the necessary electrical components. First, we have covered the optical components required to construct the spectrometer and then provide the details to convert the spectrum into information readable on a portable computer. Then we have shared the components and parts that will be used for the illumination system. It should be emphasized again that the SHS design has been determined to be unable to produce strong Fizeau fringes we need to produce the spectral characteristics of our chemicals due to the detector limitation as well as potential etendue mismatches from component to component, especially at the fiber input side of our system. This paper will describe the SHS components and design, but keep in mind that the Czerny-Turner is what was ultimately used for our Raman measurements.

3.4.1 Spatial Heterodyne Spectrometer Components

The optics components in detail will be discussed in this senior design project will be discussed in these few topics. This is an important topic to discuss to show how the final product was designed and the processed to get to that. To acquire accurate and exact measurements, optics is essential to the design of a spectrometer, especially in the choice and placement of optical components.

The scattered light from a sample will contain a variety of frequencies of light. Some of the light will consist of photons emitted from the laser that has a 532 nm wavelength. This laser has been provided to us for our project. Note that selecting this laser of this wavelength will determine the spectral range of our spectrometer since the scattered photons will shift to frequencies that are higher in the NIR region of the electromagnetic spectrum based on the principles of Raman spectroscopy. The other frequencies of light will largely consist of scattered photons that are frequency shifted. These are the Raman signals that was discussed previously in the research section. Therefore, the fiber that we use to carry the signals to the spectrometer must be able to carry light of wavelengths in near infrared from 532nm and higher.

Using a fiber can enable the user to collect the light efficiently, although there may be slight losses throughout the fiber, but also to place the spectrometer more conveniently in locations outside of the well plate reader in which the samples are placed.

This fiber will connect to a fiber collimator via an SMA connector. The fiber collimator is used to ensure that the beam spot size isn't diverging or changing shape throughout the spectrometer. The beam of light consisting of the laser signal as well as the Raman signals also must be expanded to fill the optics, particularly the gratings.

A VIS beam expander is required and must support wavelengths beyond 532nm. Since the selected fiber collimator contains a lens with an aperture of 4mm, a beam expander that scales the beam size by 3 times is needed to fill the optics as best as possible.

The sizes of the optics in the spectrometer have been selected to be 12.5mm. There are several reasons for this. One, the spectrometer is desired to be compact. Two, the size of the optics can have rippling consequences of the performance of the spectrometer.
When designing the spectrometer, there is a bit of a tradeoff between focusing between the resolving power, which determines the resolution of the spectrometer, and the spectral range, or the range of wavelengths that can be imaged upon the camera/detector. If you want to perform Raman measurements with as many samples as possible, some with potentially large frequency shifts, a large spectral range is desired. However, the spectral range is inversely proportional to the resolving power. If I choose a certain size of optics, this may potentially increase the resolving power and improve the resolution of the system. The relationship is illustrated in the equations below.

$$R = 2 \times w_{optics} \times g$$
$$SR = N \times \frac{\lambda}{2 \times R}$$

R is the resolving power, w_{optics} is the width of the optics, g is the groove density in lines per mm, SR is the spectral range, N is the number of pixels across the detector, and λ is the Littrow wavelength. There is a constant of 2 in front for the resolving power since we are considering two gratings in our system.

The Littrow wavelength is the wavelength used in the Littrow configuration. The Littrow configuration for our spectrometer is a configuration in which the first order of diffracted light is sent directly back along its path of incident propagation into the beam splitter. In other words, the angle of incidence is equal to the angle of diffraction for the first order.

The Littrow wavelength can be set to any value depending on the application, but for our cases it is appropriate to set it to the excitation wavelength value, or the laser wavelength of 532nm. Since it's the first order that's being sent back into the system, other orders need to be sufficiently blocked and kept out of the arms of the SHS. Light at the Littrow wavelength will never cross and thus will not interfere in a manner that produces an interference pattern. However, all the other wavelengths will produce the interference pattern that is determined by that band's distance from the set Littrow wavelength.

The equation that describes the grating angle in our spectrometer is as follows.

$$\frac{1}{\lambda}(\sin(\alpha) + \sin(\beta)) = \frac{m}{d}$$

In the Littrow configuration, $\alpha = \beta$. *d* is the groove spacing, and m = 1st diffracted order. Therefore, the Littrow angle, θ_L is:

$$\frac{2}{\lambda}\sin(\theta_L) = \frac{m}{d}$$

$$\theta_L = \operatorname{asin}\left(\frac{\lambda \times g}{2}\right)$$

 λ in this case is the excitation wavelength. Note the design of the spectrometer will be described later. Here we are just describing the equations necessary to understand the selected parts. Once the desired Littrow angle is calculated, a grating can be selected. This grating needs to be efficient at diffracting the laser wavelength, or in other words have a blaze wavelength of 532nm. Again, it should be noted that all optics that transmit, reflect, or diffract light should be coated to support wavelengths at 532 nm and beyond. The diffraction grating is a crucial component of the spectrometer because it directs light into the system where it is needed and allows for high resolution.

Back to the size of the optics. Notice that the size of the optics is linearly proportional to the resolving power, and thus the resolution of the spectrometer. If small optics are chosen, then the overall size of the spectrometer can be reduced, which is a part of our requirement specifications. However, this means we sacrifice the resolving power, but increase our spectral range. Choosing gratings with sufficient groove density can compensate for this, however gratings with too high groove density can result in a larger Littrow diffraction angle as well as reduce the spectral range. This is what is meant by tradeoff between resolving power and spectral range. All of this in the context of keeping our spectrometer size small. Consequently, we have chosen gratings with groove densities of 300 lines/mm.

In this project many detectors have been looked at through optical websites to see which one would be the best one for our project. A good detector for spectroscopy is essential because it will ultimately show the results of what you want to measure. In this case of our senior design project, it is contaminant in water.

Now considering the spectral range. One thing that we can considering a detector with many pixels. However, this detector needs to be able to image wavelengths above 532 nm with reasonable efficiency. The detector that we have currently selected is an IDS-Eye 3860-M-CP camera. Though its detector is only about 20% efficient at the wavelengths of interest and has an integration time of about 2 seconds, a solution would be to take multiple measurements of the spectra and scattered light at the highest integration time and sum them together while filtering out the laser wavelength signal for scaling purposes. This detector has a 2D array progressive scan CMOS with 1,936 pixels across the horizontal direction. For our design, we would just like to be able to detect the presence of contaminants and since we'll be measuring select samples, Raman peaks of interest may not necessarily overlap.

While we prefer high resolution and resolving power, producing our spectrometer to achieve this would sacrifice the spectral range. We are interested in detecting a variety Raman signal from several samples, so a larger spectral range is preferred.

With λ fixed and balancing out the width of the used optics and the groove density, using a detector with a reasonable number of pixels can increase our spectral range as per the formula seen previously on page 23.

Finally, the beam splitter is used to split the incident collimated light into the system as well as recombine the first diffracted order light to produce the interferogram that we are measuring. The interferogram has the spectral information encoded within the variance of the fringes that is imaged. Half of the light is reflected towards one of the gratings, while the other half is transmitted to the second grating. This beam splitter needs to be coated to be efficient with wavelengths used in the spectrometer.

The transmitted light reaches the beam splitter where it reflects towards the detector, while the initially reflected light is transmitted to the detector. This is the basic idea behind a 50/50 beam splitter. The light is recombined at the beam splitter and the resulting fringes are projected to the detector.

Again, light set to the Littrow wavelength will not produce the interferogram, light all other wavelengths will produce the unique interference pattern based on the band of wavelengths distance from the Littrow wavelength. In other words, these wavelengths are *heterodyned* around the Littrow wavelength and resolved by the SHS.

$$f(cm^{-1}) = 4 \times (\sigma - \sigma_L) \times tan\theta_L$$

It is convenient to describe frequency shifts in inverse centimeters, or wavenumbers, to show how far the Raman peak or band has shifted by the laser wavelength because after all we are identifying the sample based on the scattered photons, the photons that are frequency shifted, *f* is the number of fringes per cm, σ is the wavenumber for any resolved band, and σ_L is the Littrow wavenumber.

Components	Quantity	Important Characteristic
Shielded Fiber PM- 780-HP	2	Wavelength Range: 780-1100nm
SMA Connector	1	N/A
Fiber Collimator	1	Lens Aperture: 4mm
VIS-NIR Beam Expander	1	Scale: x3
VIS-NIR Aspheric Lens	1	Wavelength Range: 600nm-1050nm
Diffraction Grating	2	Groove Density: 300 lines/mm

		Blaze Wavelength: 760nm
Monochrome Camera	1	Format: 1/2.8"

 Table 1 – Spatial Heterodyne Spectrometer Components

3.4.2 Raman Illumination System Components

A laser is a main component for a Raman based spectroscopy project. The wavelength of the laser was discussed very heavily in regarding what samples we could measure with it. The two wavelengths that was discussed was 532 nm and 735 nm laser. Ultimately, the 735 nm laser was picked because it has benefits that the 532 did not. The benefit of a 735 nm laser is that I can help reduce fluorescence interference since this is a problem in Raman. This wavelength has a lower excitation energy than other wavelengths that can be used. A notch filter is used for the laser to not show the excitation wavelength which stops at 532 nm. This filter will help focus in on looking at the spectral range of the samples will be using in the project.

The laser is also a part of the illumination system. In Raman spectroscopy, the illumination part is responsible for providing a high intensity monochromatic light source in which excited the sample and generated the Raman scattering through the sample. The laser wavelength used in Raman is typically in the visible or near-infrared. For this project, then laser wavelength will be near-infrared range.

The illumination part of most Raman systems uses various filters and polarizers to remove any unwanted scattering and to ensure that only the Raman scattered light is detected. The illumination that was decided on was to use a single tight focus lens to collimate the laser beam onto the samples. Since the laser will be moving with an electro-mechanical arm the laser needs to be focused correctly on the samples every time depending on the situation. The system will use a fiber, laser, and a tight-focus lens to illuminate the samples. The laser will be coupled into a single-mode fiber to provide a stable and collimated beam.

The shielded fiber is a polarization-maintaining fiber that is designed to provide high-power handling capabilities while maintaining polarization stability. The shield in the fiber provides additional protection against environmental factors such as mechanical stress, and temperature changes. Since, the Raman spectroscopy required a relatively high-power laser source to generate a strong Raman scattered signal. The main reason of this for this shield is to improve quality and reliability of the measurements will we get from the spectrometer, particularly for the samples that we have be using. The illumination part is critical part of the Raman spectroscopy system for generating high-quality Raman spectra that will come out of a GUI. Many different components need to be carefully considered to get the best.

A fiber collimator is used to efficiently couple light from the optical fiber into free with minimal loss and minimal changes in bean quality. An achromatic fiber collimator is a type of collimator that is designed to minimize chromatic aberration, which can cause the beam to become unfocused and distort the spectral lines in the Raman spectrum.

The accuracy and resolution of the spectral lines in the Raman spectrum can be enhanced with the use of achromatic fiber collimators, which makes them particularly valuable in this field of spectroscopy. Raman spectroscopy relies on the detection of minute alterations in scattered light frequency, which are brought on by interactions between the light and the vibrational modes of the sample molecules. It can be challenging to reliably detect these frequency shifts if the beam is not well-focused and stabilized because they are often very small, on the scale of a few cm[^]1.

By adjusting for chromatic aberrations that may occur owing to light dispersion in the collimator, achromatic fiber collimators aid in reducing the distortion of the Raman spectrum's spectral lines. This may be beneficial. Overall, the accuracy, resolution, and sensitivity of Raman spectroscopy measurements can be enhanced with the employment of an achromatic fiber collimator. This can be especially crucial for applications that need for high levels of precision and accuracy, such the detection and measurement of minute components in intricate samples.

Component	Quantity	Important Characteristic
Notch Filter	1	532nm
VIS Laser	1	532nm
Shielded Fiber PM-780-HP	2	Wavelength Range: 780-1100nm
Emitting Fiber	1	Large Numerical Aperture
Achromatic Fiber Collimator	1	Focal length TBD
Raman Probe	1	

 Table 2 - Raman Illumination System Optical Components

3.4.3 Temperature & Humidity Sensor Components

As we have been developing a printed circuit board to aid the spectrometer in this project, we have been sourcing for SMD (Surface Mount Device) components that will go into the bare board. Since these are main functionality devices, various other components are going to be introduced to support the stability and proper functioning of the sensor, such as resistors, voltage regulators and capacitors. These supporting components will be talked about later in this section as we dive deeper into the specifications for these sensor components. The way we have analyze and pick components is by going through datasheets and comparing not only their capabilities but also their requirements such as voltage ratings, current drawn, as well as determining the supporting components based on this.

3.4.3.1 SHT33-DIS-B2.5kS

The SHT33-DIS-B2.5kS device is a high-precision digital humidity and temperature sensor manufactured by Sensation. It is based on the latest CMOS technology, which combines the sensing, signal processing, and calibration data on a single chip. This device shows exceptional performance in terms of accuracy, long-term stability, and low power consumption based on the datasheet.

The component measures relative humidity (RH) using a capacitive sensing element. The electric constant of the polymer dielectric layer in the sensing device changes with the water content in the surrounding air which in other words is humidity. As this humidity increases, the capacitance of the sensing element increases, which is then converted into a digital signal representing the relative humidity creating the signal that we need.

On the other hand, using a bandgap temperature sensor, this component determines the temperature value. The bandgap sensor consists of a temperature-dependent voltage reference, which is proportional to the absolute value. From this analog element and voltage, the temperature sensor output is then made digital and calibrated to provide highly accurate temperature readings.

For integration of this sensor onto the printed circuit board system, several supporting components are needed as previously stated: A microcontroller plays the biggest role in communications and overall functionality of the system, and it is necessary to communicate with the sensor, process the data, and control other system components. The microcontroller should support I2C communication, as this component uses the I2C protocol for data transmission so it would be a requirement going into microcontroller selection. The I2C protocol calls for these communication lines (SDA and SCL) to have pull-up resistors to ensure proper communication between the microcontroller and the sensor.

The SHT33-DIS-B2.5kS sensor operates at a voltage range of 2.15 to 5.5 V, so an appropriate power supply followed by a voltage regulator is necessary to provide a stable voltage within this range. Since the voltage supply that we are looking into is much higher than these ratings (12V) we have need voltage regulators to step down the voltage without affecting much current drawn. All these components require various coupling capacitors which help reduce noise and maintain a stable and reliable signal. Regulators as well as capacitors and resistors will be explained further into this section.

3.4.3.2 SHT40-AD1F-R2

The SHT40-AD1F-R2 is our second option for a device that combines temperature and humidity in one single chip. It is also a Sensirion-made device with similar functionality and accuracy as the SHT33-DIS-B2.5kS. This component also uses the I2C protocol for communications in data transfer of the digital signals it receives from its sensing elements. A couple of differences is that it lacks two pins which are the Reset and Alert pin which primarily reset the timer, functionality of the data transferring as well as data collecting and sending an alert signal when levels pass a certain threshold as SHT33-DIS-B2.5kS does, respectively.

The I2C protocol is dependent on a microcontroller as well that would communicate with the SDA/SDL pins of this chip which should be joined by pullup resistors. The datasheet provides us with a couple sample codes for the data transferring between these two components that we have keep in mind when programming our MCU and overall functionality of the board.

One of the principal reasons why this part would be selected over the already mentioned sensor is that this one comes at a much cheaper price, which falls in the range of about three times as cheaper as its selection competition. One of the primary reasons we see for this is that this chip has a much simpler functionality as it comes with a smaller number of pins. Another difference to keep in mind is the voltage rating. The rating range is much smaller in this device, showing from 1.08V to 3.6V for normal operation so higher accuracy for voltage regulators would be much more essential because of this aspect to not damage any aspects of the chip or simply keep the reliability intact.

3.4.3.3 HIH6030-021-001

The third and final option in temperature and humidity sensors is the HIH6030-021-001 which is a high-performance temperature and humidity sensor developed by Honeywell. It is attractive for our design due to its high accuracy, and low power consumption making it suitable for various applications, such as HVAC systems, weather stations, and smart home automation systems. The features for this component are the temperature measurement range: 0°C to \pm 100°C with an accuracy of \pm 1°C and the humidity measurement range: 0% to 100% relative humidity (RH) with an accuracy of \pm 4.5%. For the supply voltage, it accepts 2.3V to 5.5V, allowing compatibility with a wide range of microcontrollers as we have been using 3.3V as a supply.

The digital output for the sensor calculations uses the I2C communication protocol which will be used alongside two 2.2kOhms pull-up resistors with the supply voltage into the microcontroller. The data is read and ready for transferring at 5ms for humidity and 30ms for temperature measurements.

This HIH6030-021-001 sensor comes in a SMD 8-pin SOIC package. The compact design and package due to its pad shaping and sizing makes it suitable for space-constrained and applications that require a lot of testing like ours as we have been testing those pins with multimeters and good pad shapes and pad sizing is critical for this. The sensor comes factory calibrated, which eliminates the need for any additional calibration during installation.

The reason the HIH6030-021-001 is the sensor of choice is due to the package it comes in as well as pins of the device as they are external and will come in very handy at the time of troubleshooting the PCB.

The specifications of the device align perfectly with what we are looking for and the I2C interface protocol to communicate with the microcontroller is ideal for us, while the price comes at a higher number, we believe implementing this package into the design instead of a DFN is worth it.

Feature	SHT33-DIS-B2.5kS	SHT40-AD1F-R2	HIH6030-021-001
Voltage Rating	2.15-5.5V	1.08-3.3V	2.3-5.5V
Current Drawn	6mA-15mA	3.2mA-5mA	.65mA
Power Cons.		~2.6uW	~
Size	2.5mm x 2.5mm	1.5mm x 1.5mm	SOIC-8
Pins	8	4	8
Price	\$9.60	\$3.12	\$12.5

 Table 3 - Temperature & Humidity Sensors Comparison

3.*4.4 Computer Options*

To be able to gather and present the data from the spectrometer, it is necessary to have a computer that can run the required software. This software should be able to gather, process, and present the data in a way that is easy to read and easy to understand. We believe the best way to do this is in the form of a graphic user interface (or GUI). Spectrometer data is relatively difficult to process and analyze so using the right software is of vital importance. However, to efficiently use the correct software, we need a computer with the system specifications necessary to run the program written by our team.

To create the GUI, we have use MATLAB as this is the language that has the lowest system requirements while also being capable of performing the complex mathematical computations required to present the data it in a way that means something to our users. Additionally, the professionals in the spectrometer field that we have talked to all recommended MATLAB as the software they used for performing similar calculations. Therefore, the computer that we use will have to have the bare minimum requirements needed to download, install, and run MATLAB app designer files.

There are a few things that must be considered when deciding on which computer to utilize for this project. We must first decide on what the requirements are for each component of the computer to create a short list of possible computers that we can use for our project. Once the short list has been created, we can move on to narrowing down that list by evaluating different factor like feasibility, implementation, cost, and size. The most important thing would be implementation since we must be able to connect the spectrometer, laser, and motor to the computer to receive the data from the spectrometer and then operate the other components at the same time. Our current design includes a USB hub that attaches to an outside computer and there may be some difficulties if we must build and connect an entire PC. The next factor that we must consider is the size of our computer. We want our system to be portable in one aspect or another. The spectrometer itself will most likely not be portable but we want to be able to use the machine and interpret the results without being anchored to the system. To add on top of the two aforementioned factors to consider, our spectrometer will have an enclosure that contains the laser, motor, power supplies, etc. (all the

things that make our spectrometer a spectrometer) so if the size of our computer is so large that we'd need to build a second enclosure then that computer would be eliminated as that requires coming up with solutions for how we have keep the two together close enough to be connected, how we have connect them, and will most likely end up being too pricey and complicated to be worth the effort. The very last factor we have consider is the price. As strange as it sounds, price is not necessarily a factor for us due to our project being completely funded by Ocean Insight. While there are limits to our funding, the cost of the part would have to be an exorbitant amount for it not to be considered.

When choosing your computer, the internal hardware components are important in that the software will not be able to run without the minimum hardware requirements being met. However, to be able to make the connections the computer must have the necessary port connections to be able to completely connect to the system. Therefore, the computer must have a mouse or touch screen, an ethernet port or Wi-Fi capabilities, and multiple USB ports. The most likely computer that will be used to operate our spectrometer will be a laptop which already has the mouse and Wi-Fi capabilities but often, but new laptops do not have as many ports.

When choosing a computer to connect to the system, a minimum of 4 USB ports and 1 ethernet port is required to fully connect to all the parts that require a hardwired connection. If the only available computer does not meet these minimum requirements, an easy method is to buy a USB hub. From there you can connect wires that make the connection from component to computer as well as any adapter that might be needed to create an ethernet connection. The most likely situation is the computer having a USB-C connection which will take an USB-C to ethernet adapter and are commercially sold for just a few dollars apiece.

3.4.4.1 Processor

MATLAB requires an Intel or AMD x86-64 processor to run download, install, and run the software (MATLAB, n.d.). Essentially, the computer that we chose needs to have a central processing unit with at least 4 cores. The reason that multiple cores are required is because most programs that are run in MATLAB perform mathematical computations in parallel quite easily. Each of these computations is performed in a thread and multiple cores are required for multiple threads.

At the very top of our list (disregarding funding) we have the AMD Ryzen Thread ripper Pro 5000 series. These processors are cutting edge with a whopping 32 cores and a clock speed of up to 4.2 GHz delivering blistering speeds to your PC (AMD, n.d.).<u>At the very top of our list (disregarding funding) we have the AMD Ryzen Thread ripper Pro 5000 series. These processors are cutting edge with a whopping 32 cores and a clock speed of up to 4.2 GHz delivering blistering speeds to your PC (AMD, n.d.).<u>At the very top of our list (disregarding funding) we have the AMD Ryzen Thread ripper Pro 5000 series. These processors are cutting edge with a whopping 32 cores and a clock speed of up to 4.2 GHz delivering blistering speeds to your PC (AMD, n.d.).Another CPU that is recommended for MATLAB and other</u></u>

engineering software's Intel Xeon processors. Another CPU that is recommended for MATLAB and other engineering software's Intel Xeon processors. The thing that makes this processor special is that they are scalable which means that you can combine multiple of these processors, and they will behave like 1 CPU, allowing for increased cores, and therefore, more threads for computations (Intel, n.d.).

The CPU that is most likely to be our choice is the Intel Core i7-8565U. It is small, light, and appears in many average laptops. It carries 4 cores allowing for 8 threads to run at once and has speeds up to 4.6 GHz when overclocked, but this can be affected by the cooling capabilities of the laptop. Important features of this CPU are that it is easily fit into a laptop (thus maintaining our portability feature), within our budget range, and runs any MATLAB processes with ease (Intel, n.d.).All these CPUs run on an x86 architecture which meets the MATLAB requirement of supporting an AVX2 instruction set (MATLAB, n.d.).

Feature	AMD Thread ripper	Intel Xeon	Intel Core i7-8565U
Cores	16	4	4
Clock Frequency	4.0 GHz	3.0 GHz	1.8 GHz
GPU	No Integrated Graphics	No Integrated Graphics	Intel UHD Graphics
Cache	8 MB L2 Cache	12 MB L2 Cache	8 MB Smart Cache
Price	\$7,000.00	\$969.00	\$409.00

Table 4 - CPU Comparison Table

In the end we decided to go with the Intel Core i7-8565U processor because it is the most cost efficient, readily available, and exceeds the requirements needed for MATLAB and any services needed for the spectrometer and its peripherals.

While the Thread ripper series is impressive and don't leave the user wanting for more speed; this processor is in the \$7,000 range which clearly surpasses our budget and puts this processor out of the question for our project. Furthermore, the issue with the Xeon processors is that they require too much space for our system and would require a new, larger compartment to hold the CPUs along with the rest of the equipment required to make our spectrometer function. One solution to this would be to purchase a second compartment that would be connected to our spectrometer and any mouse, monitors, or keyboard. However, this would essentially mean we would need to build a PC whose sole purpose is to run the spectrometer that it is attached to. This is far too expensive, complicated, and removes the portability aspect of this project.

3.4.4.2 RAM

To appropriately run MATLAB our computer first has the necessary storage space to be able to store all the files and software space on the computer. The manufacturers site states that they require a minimum of 4 GB of RAM, but 8 GB is recommended. RAM is easily one of the most common specifications for any software to have a minimum requirement. This is since RAM is very important for any process occurring in a computer. The purpose of RAM is to give applications a place to store and access data on a short-term basis. It stores the information your computer is actively using so that it can be accessed quickly when running any time of programs that you ask it to run (Crucial, n.d.). This means that any data that is received and must be manipulated in some way is stored in the RAM while the software completes its purpose. This is crucial for us because the only thing the user really sees is the data that the computer performs calculations and displays on a GUI. For that reason, it is quite easy to see that we would want to meet the 8 GB recommendation to aid the multithreaded processing our computer will be performing when running our MATLAB code.

Another factor we must take into consideration when deciding the type of RAM to incorporate is the frequency that our computer runs at. The reason we must take this into account is because there are different speeds that a computers motherboard runs at. The frequency of a motherboard is what we call the alternation of high and low voltages that a motherboard cycle between. The rate that these voltages cycle is directly proportional to the clock frequency of the computer. If we are to choose a RAM frequency that runs too quickly some of our RAM frequency will go to waste as the computer, simply cannot keep up with the RAM and the RAM is forced to limit its speed. However, if we are too conservative with our choice and choose a speed that is too low, we have limited our computer's performance instead. Luckily, we know what the frequency of our motherboard runs at because we know that the clock speed of our processor (chosen in section 3.3.4.1 above) is at least 1.8 GHz up to 4.4 GHz. With speeds of that level, we do not need to worry too much about buying RAM that could be too fast.

The final consideration for choosing RAM is the type of RAM. The types are DDR, DDR2, DDR3, and DDR4. Thankfully, DDR and DDR2 are obsolete these days and do not need to be considered. DDR3 and DDR4 are the only two types that we need to consider so we should look at the few differences between the two. DDR3 is older but still considered a standard (Moglix, n.d.). DDR4 is (obviously) the newest standard and therefore cost more money to buy but it comes with much higher frequencies. The frequency of DDR4 begins near the maximum frequency that DDR3 achieves and has a better value-per-dollar than DDR3. Additionally, DDR4 comes with more capabilities than DDR3 even when the two have the same

frequencies. Overall, DDR4 is clearly the better choice for our computer, and we have only had to worry about the price when deciding on our RAM since we also do not need to worry about the frequency and RAM is generally does not take up a lot of space in a computer system.

	DDR1	DDR2	DDR3	DDR4
Frequency	133-200 MHz	266-400 MHz	533-800 MHz	1066-1600 MHz
Voltage	2.5 V	1.8 V	1.35 V	1.2 V
Data Rate	266-400 MT/s	533-800 MT/s	1066-1600 MT/s	2133-3200 MT/s
Transfer Rate	2.1-3.2 Gb/s	4.2-6.4 Gb/s	8.5-14.9 Gb/s	17-21.3 Gb/s
Memory Clock	133-200 MHz	133-200 MHz	133-200 MHz	133-200 MHz
Price	N/A - obsolete	>\$20	\$10-\$20	\$15-\$40

Table 5 - Table comparing RAM options.

3.4.4.3 Storage

The final component that MATLAB requires a minimum capacity to run their software on our computer is to have the necessary storage space to be able to store all the files and software space on the computer. The manufacturers site states that they require at least 3.8 GB for just MATLAB but up to 23 GB for all products related to MATLAB. 23 GB is quite a lot of storage for most cheaper computers without paying to upgrade the storage. One solution to this would be to buy a separate external hard drive that would contain all the MATLAB files and would connect to our computer through USB. This is a simple \$20-\$30 solution that does not require much effort other than making sure that the hard drive is securely removed and that the drive is connected when we are using the software.

Preferably, the better solution would be to just download what we need which would just be the 3.8 GB required for MATLAB itself.

Now that we know exactly how much storage we need for the installation, we need to figure out which hard drive we want for our computer. Before finding exact products, we must decide on an SSD or an HDD. SSD/HDD are types of hard drives in a computer, and each have their own advantages and disadvantages (Tom Brant, 2022).

	SSD	HDD
Fastest	Х	
Longest Lifespan		Х
Highest Cost	Х	
Most Durable	Х	

Table 6 - Table comparing SSD and HDD characteristics.

The most attractive difference between the two is that an SSD is much faster. The reason for this is that an HDD is a mechanical hard drive that stores data on its disk, and something called a "head" moves over the disk to read the bits that contain the data. In comparison, an SSD stores data electronically on "cells" that the hard drive can access much faster than HDD. The SSD is also lighter, uses less energy, and more durable than an HDD for one simple reason. An SSD has no moving parts. The fact that an HDD must move around to read the data means that it takes longer to find and read the data, the "head" can easily be damaged from a drop, and it drains more of the battery. However, due to the SSD being having more advanced technology it comes at a much higher price point; about two times as expensive as an HDD for the same amount of storage. Due to this price point, the memory that we choose we be determined on price point, availability, and ease of implementation.

Now that we know the possible hard drive characteristics, we need to determine which hard drives we want to use. We know that we need at least 8 GB of storage on our hard drive however that it is quite limited for any other applications we might want to use on that computer. While we could simply add a 16 GB USB drive that would be constantly attached to the computer it would be easier and probably not much cheaper to simply buy a hard drive with 16 GB. Preferably, we would also want an SSD drive despite how much more expensive they are since they are best

used for engineering professionals (Tom Brant, 2022) (we may not officially be professionals yet, but this project makes us all feel like we are). Similarly, to the RAM, when it comes to hard drives there are no model numbers or specific prices but rather, we go online, choose a brand, whether we want SSD, HDD, or both, and how much storage we want. From there we have decided which we want to buy based basically off price and the size of the hard drive as those are our only 2 limiting factors.

3.4.4.3 Operating System

Another important aspect to consider when choosing what kind of computer, we want for our spectrometer is the operating system. Operating systems are usually overlooked when it comes to choosing a computer, but the operating system will decide how easily you are able to efficiently use your computer. Some factors to consider include which brand; Linux, Windows, or Mac, which version of that operating system, and which operating systems does MATLAB support.

First, we must choose which operating system would be ideal for our system. Out of the 3 choices, Linux would be least ideal as there are not many computers that come preinstalled with Linux meaning that we would need a virtual machine. Virtual machines are not terrible to use but using one adds another level of abstraction that we may not want to add. Our next option is Windows; Windows is the most common operating system used for MATLAB and general engineering practices. However, Windows 11 has a few cons that could become issues. The most important one is that Windows 11 has hardware requirements that make it more difficult to use older (and thus less expensive) equipment. The 2nd more relevant issue is that Windows 11 requires the user to sign into a Microsoft account to be able to use the computer. This could be an issue as not everyone will want to sign up for Microsoft. For that reason, we consider using Mac instead. Mac OS is the preferred operating system for programmers because it is built on top of Unix and most web and database servers are based on Unix (The PyCoach, 2022). However, MacOS has a more rigid file system compared to Windows. Furthermore, Windows allows for the creation of executable files. This is very useful for selling the product because instead of requiring the user to download and pay for MATLAB (and MATLAB is not exactly a cheap software) we would be able to send the buyer an executable file of the program along with the system. This executable file contains all the data, code, and files required to run the program without needing the full version of MATLAB.

After some deliberation we have chosen Windows 11 as our operating system. The reason we chose Windows is because that is the operating system that we are all most familiar with. And while there may be some discrepancies with the ease of use for Windows 11 it is the most recent version of Windows and most likely already installed on the computer we choose. Furthermore, using the most recent version of Windows also means that we do not have to worry about our computer not having support for the minimum instruction set required to run MATLAB. This is because instruction sets are always backwards compatible. There are standards for developing computer architectures and instruction sets for operating systems and one of those standards is that new, updated instruction sets can always have new features, but they can never remove features. Thus, if we have the most updated operating system installed on our machine then we are guaranteed to have the most updated instruction set and, therefore, are. guaranteed to have support for the AVX2 instruction set required by MATLAB to run.

	Windows	MacOS	Linux
Release Date	1985	1984	1991
Availability	Default on most computers, requires a license	Reserved for Apple computers	Free, open-source operating system.
File Structure	Hard drive is divided into partitions with folders inside	All apps and user-data are stored in one section of the hard drive.	Tree-style storing; files are added at the top of the hard drive as they are created
Registry	One master database stores all logins, settings, and preferences	Logins, settings, and preferences are stored in a series of. plist files	No exclusive registry, settings and data is stored with the related programs.
Interface	Gained the ability to be changed with the production of Windows 8	Always been possible but requires some system management	Very easy, no installations required
Terminal	Basic terminal prompt and functionalities	Basic terminal prompt and functionalities	Basic terminal prompt and functionalities. Vital for Linux as most functionalities require a command to be run in the command line of the terminal

Table 7 - Table comparing operating systems.

3.4.4.4 Computer Selection

After doing the thorough research in the sections above to determine what would be the ideal computer for our project, we were able to narrow it down to three computers. We realized early on that building a separate PC with the most ideal specs po12ssible was way too expensive and time consuming as we would have had to not order a whole separate enclosure for the PC but also all the supporting hardware for RAM, a CPU, and a hard drive. Furthermore, there would be some real issues created when we tried to connect it to the spectrometer itself to gather all the data in a way that wasn't messy and still looked clean and professional enough to sell to consumers. To top it all off, we would also have to buy peripherals for the PC so that the user would be able to use the PC but that would force the user to be attached to the spectrometer to do any type of work with the data. This would eliminate any possibility for the user to be able to analyze and do something with the data without saving it and sending it to another computer or dragging the spectrometer to somewhere convenient where the user can access the data as needed. Neither are ideal and for that reason we decided to start looking into laptops. This would allow us to use a simple ethernet connection to connect from the spectrometer to the computer while the system was running and then the user would be able to carry the laptop to wherever they desire to continue working on their project.

After having narrowed it down we decided to first start looking for any laptops that we already had that also met the qualifications for MATLAB. This would greatly reduce the price and make things that much easier for us to immediately start working on the software aspect of this project. Additionally, we also do not need to provide a computer with the system when we sell it as most newer laptops easily meet the qualifications to run MATLAB so all we would need to supply would be the spectrometer and the software required to run the machine. While doing so we narrowed it down to two laptops and a single board computer. The single board computer was supplied to us by Ocean Insight, and we realized that we could plug this board into the computer, it would run all the necessary programs through a series of executables, store the data, and then be plugged in at any other monitor to analyze the data. The specs for each are down below.

	Latte Panda	Dell XPS 13 9315	ASUS ZenBook Q526FA
Processor	Intel Atom x5- Z8350	Intel Core i5- 1230U	Intel Core i7-8565U
Number of Cores	4	8	4

Storage Type	HDD	HDD	SSD-HDD Hybrid
Storage Capacity	64 GB	256 GB	1128 GB
RAM	4 GB	8 GB	16 GB
Operating System	Windows 10	Windows 11	Windows 11
System Type	64-bit	64-bit	64-bit

Table 8 - Table comparing computer options.

From the table above we can see that ASUS ZenBook Q526FA is far and above the better choice. Although the Latte Panda could be used later as an extra feature, but it is simply not worth the effort to try and integrate that into our design plans. The Latte Panda is a single-board computer which means that it does not have all the capabilities of a regular computer with 4 cores and one of those limitations is that it does not have the capability to perform multithreaded operations. The final reason why we didn't choose the Latte Panda is because it would be much easier to simply attach a laptop to run the system as that allows for customization of the settings when running the spectrometer. Consequently, we have narrowed down our choices to Dell and the ASUS. Now, even though the Dell has more cores the ASUS has more characteristics that we are looking for. The ASUS has more RAM, more storage capacity, and a dual SSD-HDD storage type. These SSD-HDD hybrids are a combination of the two systems that allows for the large storage capacity of the HDD while also the rapid performance of the SSD when booting up or running the most used applications. Overall, the ASUS ZenBook Q526FA is the better choice since it rivals the other choices in all aspects except for number of cores in the system but our team has decided that that it is a negligible advantage when compared with the many advantages that the ASUS offers on top of the i7-8565U also being a more recently developed central processing unit.

3.4.5 Microcontroller Options

Microcontrollers are the living heart of a PCB design and an electrical project overall. Our design will need various connections ranging from voltage steppers, external board connections for devices such as the DC fan, latching device and PC, sensors, and the innumerable other components supporting our overall design. The one way to make sure our PCB is actively communicating, sending, and receiving the correct signals is by adding a microcontroller. In order to relay the correct power and signals to the various components throughout our system, we have to design PCBs and buy the appropriate hardware and we also need to use microcontrollers to interpret and communicate the signals that the user sends to the system when using the software installed on their computer like in the case of CCS and UART connection that will serve as the bridge connecting us and our printed circuit board.

Many manufacturers have distinct types of MCUs that may serve from different purposes such as motion and general-purpose microcontrollers which is what we have be diving into in this microcontroller device selection section. There are many things to keep in count when selecting a microcontroller which may be voltage ratings, number of GPIO pins which stands for general purposes input and output and are the leads of the device to be programmed through the device's internal circuit and the software the microcontroller is based on. The software side is also a big feature to keep in mind when doing selection as different manufacturers may have different syntax, applications and characteristics when programming a microcontroller. For this reason, we have been focusing on the Texas Instruments' and STMicrocontrollers' MCUs as they are what we have most experience in and most popular in the market, respectively.

3.4.5.1 MSP430FR6989

The MSP430FR6989 is our main choice of microcontroller from Texas Instruments, by offering a great combination of performance, power efficiency, and a great set of peripherals we determine that it could be an excellent choice for our design, given its features and characteristics that make it perfectly, if not over capable, of the requirements in our electrical design.

This microcontroller features a 16-bit RISC processing unit, which enables efficient processing and at a low cost of power operation. This MCU has up to 128KB of non-volatile FRAM that provides faster write speeds, lower power consumption that will serve for the speedy functioning of the overall design as it will be the main way of communication with the many critical components in the printed circuit board as well as the external devices through the means of communication protocols and an integrated USB circuit.

The MSP430FR6989 is designed for battery-powered applications, with multiple power-saving modes that minimize power consumption during operation and idle periods but as our PCB will not be powered by a battery this is an extra feature that we may not use much of other than aiming for optimal performance. It offers up to 74 GPIO pins, allowing for a great number of integrations with various sensors, and other external devices. Another reason this is our choice of microcontroller is that the MSP430FR6989 includes all the communication protocols in addition to other peripherals within its design that will be used such as

UART, SPI, I2C, timers, ADC, DAC, and comparators, that provide flexibility in implementing the different functionalities to be used in the project.

To use the MSP430FR6989 in our project, a set of measures must be taken for its proper functioning. The set-up of the development environment is done by the appropriate software tools which in our case will be CCS, Code Composer Studio, alongside the Launchpad development kit, which includes an onboard debugger and programmer. This combination of hardware and software will be implemented into our PCB by the required connectors between the devices that will communicate via TI's Spy-By-Ware feature. The simplicity of using this feature was the biggest step in choosing our microcontroller as a lot of money and extensive connections and headaches may have a raised if having to program the board through JTAG as we would need the MSP430-FET that costs around \$100.

3.4.5.2 MSP430G2553

MSP430G2553 was our second TI option as we also interacted with it at UCF in intro to C class for the final project. It serves highly similar connections and characteristics as the FR6989, but we decided not to go with this microcontroller as it is much smaller by less GPIO pins to make use of, and we would rather overdo it than miss pins as soldering and resoldering MCUs into and from a PCB is a highly risky process for the safety of the device and board. A highly attractive feature, however, was the ability of being able to switch out the microcontroller from the development board as it comes in a through hole package which would make the programming of the chip much faster.

3.4.5.3 STM32G431C6T6

The STM32G431C6T6 is a microcontroller developed by STMicroelectronics from the STM32G4 family. Because of its size it is ideal for designs with multiple signals which in our project is a requirement when picking microcontrollers due to the number of signals that will be shown by many of the critical components in the design. The MCU is based on the Arm Cortex-M4 core, which features floating-point unit (FPU) and digital signal processing capabilities. This core runs at a frequency of up to 170 MHz The STM32G431C6T6 has 32KB of flash memory used in data storage and program execution.

The MCU comes with a variety of analog ports, such as two 12-bit digital-to-analog converters (DACs), three 16-bit ADCs, and a 12-bit successive approximation register (SAR) ADC. These ports enable the microcontroller to interface with various analog signals in real-time and perform signal processing tasks. It also supports multiple digital communication interfaces, including I2C, UART, SPI, and USB, which is one of the main reasons it is an option to be one of our microcontrollers. USB, UART, and I2C communication protocols will prove to be key when communicating the components, we use for spectrometry signals. Just

like Tis microchips, it provides a range of timers, advanced control timers, and lowpower timers, which enable precise control and measurement of time-based events. The use of clock signals will be essential and a throwback as we acquired some of these skills when taking Embedded Systems at the University of Central Florida.

The microcontroller is designed with low-power operation in mind and supports various low-power modes, such as Sleep, Stop, and Standby modes, which help to reduce power consumption when the device is not actively processing tasks. STMicroelectronics provides a comprehensive set of software tools, and libraries such as the STM32ProgCube software development platform, which will aid in the development of applications to be used within our project.

The capabilities of the STM32G431C6T6 seem to align very well to the needs of our spectrometry project. The most attractive features coming from the microcontroller are the communication protocols supported that will be essential for the processing of the sensor, interlock, and camera signals to be communicated with the PC. The size of the microcontroller, as well as its padding are features to not be overlooked at as troubleshooting may be a simpler step.

3.4.6 Power Supply Options

Microcontrollers such as the MSP430, use voltage levels of 3.3 and 5.0 volts. The power supply will be integrated within our breadboard to a certain degree. Working with 120V mains electricity is too dangerous for this project, given that we must test it and make sure it works. The equipment in the lab has power supplies but the power supplies in there only go up to 30 volts DC, and the AC power supplies give a maximum of 20 Volts peak to peak. Using a 24-volt power supply that we can then step down is much safer and feasible. We can then step down the voltage as needed to provide the voltage level for our board and other auxiliary components such as our temperature and humidity sensors.

This power supply will also be for the safety interlocks as well, so we can make sure that the entire safety system will be properly always working. Our laser comes with an integrated power supply, and so will our computer. Those components will therefore not be put under consideration for the selection of the power supply.

3.4.6.1 Mean Well EDR-120-24

The EDR-120-24 is a 24-volt power supply that can deliver up to 5 Amps of current. It has two negative and two positive terminals, which means it could feed 24V into our buck converter integrated into our MCU, while also feeding power into the safety interlocks. A bonus to this power supply is that I can be latched onto industry standard DIN hardware rails, this improves serviceability and modularity. If the power supply fails, it can be replaced by any equivalent unit that can be mounted

on DIN rails. DIN rails are simply a common industry term for IEC/EN 60715 mounting systems that allow us to mount a host of things into the enclosure for our spectroscope. The mean well EDR-120-24 is also cheap compared to the other options that we are looking at, but this notable comes at the cost of size. The EDR-120-24 is large compared to the other power supplies, being almost twice to three times the size of the others. This would be an issue if we were to be looking at a more compact design, but the enclosure is big enough to fit it.

3.4.6.2 XP Power LCW100US24

With an even broader input voltage range, the LCW100US24 provides even more flexibility for input power, taking input voltages from 85VAC to 305VAC. The power supply also gives us a maximum 4.5 Amps of current at 24 volts. This is slightly less than the EDR-120-24, however it comes in a much smaller form factor. One thing that makes it less desirable is the lack of DIN rail mounting capability. Other issues it the lack of multiple outputs, although connecting two loads onto the same power supply is possible, we would like to avoid this if possible due to current back feed issues that it could introduce in our circuit. This would require the introduction of fuses to ensure that the current does not go to places where it should not be. This problem can cause damage to our parts, which again, we would like to avoid.

3.4.6.3 RECOM POWER RAC25-24SK/480

The RAC25-24SK/480 built by RECOM POWER also gives us 24 volts of output, however the current for this power supply is the lowest of them all. Giving only 1.04 ampere, this however should be enough to power our microcontroller board and safety systems without trouble.

This power supply is also able to be mounted on DIN rails. The single output channel also makes it difficult to pick compared to the other power supply options. It is also extremely small, which will make it the leading candidate if we were to run into space issues.

3.4.6.4 Power supply comparison table

	Mean Well EDR-120-24	XP Power LCW100US24	RECOMPOWER RAC25-24SK/480
Output Current	5A	4.5A	1.04A
Power	120W	100W	25W
Output Voltage	24V	24V	24V
Operating Temperature	-20C to 60C	-30C to 70C	-40C to 90C
Ripple & noise	120mVp-p	150mVp-p	100mVp-p
Input Voltage	Min:90VAC Typ:115/230VAC Max: 264VAC Min:127VDC Max:370VDC	Min: 85VAC Typ:115/230VAC Max: 305VAC Min: 120VDC Max: 430VDC	Min: 85VAC Typ: 115/240VAC Max: 528VAC
No load power consumption	Unspecified	500mW	300mW
Price	~34\$	~30\$	~35\$
Additional Specifications	DIN rail mounting support.	Small form factor, has holes mounting mechanism.	Completely sealed and built for adverse conditions.

Table 9 - Tabulation of power supplies comparing various performancecharacteristics and parameters.

Comparing the power supplies, the recomposed unit looks like the least worthy candidate. Having 1 amp of power would be fine, but since additional safety systems may be added in the future, we would prefer to avoid that. In addition to the maximum output current not being suitable, the completely sealed nature of

the device means we would not be able to easily mount it in our enclosure. The XP power unit alleviates this concern, but since the mounting holes are not standardized, this might cause troubles in the future, should the power supply fail and require maintenance. Another issue with the XP power unit is that the ripple current being higher than the mean well unit, that extra 20mVp-p of ripple may not sound like a lot but being compared to another unit with standard mounting hardware, it becomes the difference maker. Half an amp of extra output current on the mean well unit finalizes the choice of power supply. The mean well EDR-120-24 ends up being our choice of power supply, the form factor makes it very easy for it to fit in our spectroscope enclosure. Standard mounting hardware also adds replaceability of the power supply, which improves repairability, which is a desirable trait for our customers, given that the spectroscope is being built for a business.

3.4.7 XY table

For this specific application we are looking for a movable table that can move in 2 directions. These are sold specifically as XY-tables for scientific use. We have been using one that can preferably hold as many well-plate samples as possible in our enclosure to maximize time spent scanning our samples. This XY-table will have to be able to hold our well plate, while also moving it to the correct sample to scan that one. Furthermore, an XY table needs a motor controller. Motor controllers and XY tables are sold separately. Buying separate controllers can be done, but compatibility must be ensured. This motor controller will be plugged into the computer and that will be the way we control the motorized XY-table. This will also allow us to adjust the location of the well plate and make sure that the laser is always calibrated to the well plate. The granularity of these tables is very good, usually moving fractions of a step on the stepper motors to move the table itself by fractions of a micron. The control and granularity required by this piece of equipment means that we must buy one instead of designing it by ourselves.

3.4.7.1 MOXY-01-100-100

Our first option for the XY table will be the MOXY-01-100-100 made by optics focus. The XY table is good for our needs. However, we have need to implement a well plate reader into it since it does not come with one standard. It uses a DB9 connector for motor control which we must use since the motors are built in, this connector is built upon the RS-232 connector which is commonly used across multiple industries. This interface however has mostly been phased out in favor of USB. The specs, however, are very good, boasting a resolution of 0.625 microns. This resolution makes it very easy for us to move the well-plate properly, given that the radius of the wells in the well-plate are around 3mm, having 0.625 microns of resolution. One downside is the travel range being 100mm*100mm. Our plan to use a 96 well well-plate becomes difficult due to the well plate dimensions being

larger than the travel range of the XY-table. This issue can be remedied by using a smaller well-plate.

3.4.7.2 ZABER ASR

The Zaber ASR series of XY tables comes with a lot of advantages. One of the biggest advantages is that unlike many other XY tables that are built mainly for microscope use, the ASR series is more adaptable as our situation could change. The ASR has additional attachments from Zaber that make it an extremely compelling option for our use case scenario. One of the attachments that Zaber makes for it is a well plate attachment, that securely holds our well plate in place during scanning and movement. This is very good in a multitude of ways. Starting with the adjustable well-plate readers, they make multiple sizes that can fit different sizes of well plates. We plan on using a 96 well well-plate for our testing. Future upgrades can be done easily using other Zaber attachments such as their multiplate attachment that can fit 6 microplates. This would allow for less downtime when it comes to switching out well-plates. In addition to this bonus, Zaber also provides the controllers needed to move the stepper motors built into this, ensuring the performance needed for our application.

3.4.7.3 PI L-731 Precision XY-stage

The L-731 Precision XY stage made by PI, is different compared to the other components, it features a much wider travel range for the X and Y axis, 200mm*200mm. The other XY-stages that we have looked at have less range compared to the L-731, having 120mm*120mm for the Zaber ASR and the MOXY-01-100-100 being even worse at 100mm*100mm. The L-731 also features by far the best resolution out of all of them, having 1nm of resolution. This resolution is useful for microscopic analysis, but the resolution is simply too much for the task at hand, 1micrometer is already more than enough precision for what we need in this use case. The super fine resolution in this case is a waste of money. Although this is not explicitly a downside to this XY table, the lack of a drive controller being included with the XY table is a negative.

3.4.7.4 Comparison Table of XY-Tables

XY Table Model	ZABER ASR	PI L-731	MOXY-01-100-100
Controller compatibility.	XMCC With autodetect	None included manufacturer has recommended list	None included or sold by manufacturer
Travel Range	100x120	205x205	100x100
Resolution	0.15625um	1nm	1.25um
Motor type	Stepper (2 phase)	DC Motor	NEMA17 Stepper motor
Max Speed	85mm/s	50m/s-90mms	20mm/s
Price	Order Dependent	Order Dependent	2739\$
Operating Temperature range	0C to 50C	5C to 40C	Unknown

Table 10 - XY-Tables comparison.

Overall, the XY tables are expensive and have very similar specifications for what they are worth. Out of the three we decided on the Zaber ASR, given that they not only provide included microcontrollers for this application, but also because their microcontrollers come included with autodetect. Autodetect allows us to bypass the programming stage for the XY table and use it through the interface provided by ZABER. Another fact that led to us choosing to use Zaber was the included accessories that they sell, such as a well plate holder that can hold our samples. Given the machining and precision required for the XY tables, and the size of the samples and well plates, producing an XY table from scratch would have been worthy of a senior design project on its own.

3.4.8 Voltage Regulators

Voltage regulators are essential components within an electronic circuit that maintain a stable and constant output voltage, for some, regardless of input voltage fluctuations or variations in current. They are widely used in many

applications, such as power supplies, and devices that require a stable power source such as the devices we are adding into our printed circuit board as they have voltage ratings ranges.

Voltage regulators act as an intermediary between the input power supply and the different circuit's components. They ensure that the output voltage remains at a constant predetermined level, protecting sensitive components from damage due to voltage fluctuations that may happen. There are two main types of voltage regulators: linear regulators and switching regulators. Linear regulators provide a simple, low-noise output but are less efficient, while switching regulators offer higher efficiency but may generate more noise. In this project, we have been choosing buck converters over linear voltage regulators primarily due to their higher efficiency, reliability, and simplicity through TI Webench. When dealing with a substantial difference between input and output voltages, buck converters waste less power as heat, ensuring that the system remains cool aiding the fan system and reducing the need for additional cooling measures which are still implemented due to the criticality of the system. The increased efficiency results in longer battery life for portable applications. Buck converters provide a smaller form factor and are often lighter compared to linear regulators, allowing us for a much more compact design. They exhibit a faster transient response, which makes them better suited for applications with rapidly changing loads.

These advantages make buck converters ideal for the system we are building. However, a good factor to keep in mind is that our project deals with many components that require high levels of accuracy and therefore, linear regulators may look like a more ideal choice as they can reduce noise level and further protect the most critical components which are the optical devices, but we believe it will not affect our system in such a delicate way and hence we have be choosing buck converters.

The process to be used in identifying the best voltage regulators is divided in the most important steps which are found to be to firstly obtain the voltage level needed by components to be powered by the regulator. This will be the target output voltage of the device. Determine the minimum and maximum input voltage levels that the regulator will receive. This will be from the main power supply but may also come from any other part of the circuit.

Estimate the maximum current that the circuit will draw. This is important because the regulator must be capable of supplying sufficient current without overheating or shutting down. The following components start with linear voltage regulators that were our primary choice before we switched to buck converters after analyzing the simplicity of the design and what we most desire which was reliability and buck converters offer that. Non-linear voltage regulators will be shown after the linear regulators. The buck converter selection was done using TI webench which simulated our desired specifications and output many design options which we then handpicked based on a balance of price, efficiency, and size, which may also fall into the category of price due to PCB manufacturing.

3.4.8.1 MAX25302BATD/V+

The MAX25302BATD/V+ is a linear voltage regulator by Maxim Integrated that has an adjustable output. An adjustable output refers to the capability of manipulating the output to the user's desire by simply following the math and choosing the appropriate resistor values to obtain the voltage that will ultimately go to the components.

A typical application circuit shows that by-pass capacitors are also needed for proper functioning of the device mainly to deal with noise and keep a stable voltage.



Figure 20 - Typical Application of MAX25302BATD/V+ from Datasheet

The math required to obtain the desired output voltage is no more complex than the voltage division equations learned in circuit classes. For even more simplicity, most of the work is already given in the datasheet.

$$R1 = R2x(\frac{V_{OUT}}{V_{FB}} - 1)$$

 V_{FB} is the feedback regulation voltage which equals 0.6V, V_{out} is set to the desired voltage. Then it is left to a matter of plugging in resistor values to find the most optimal ratio between them to solve the equation at V_{out} .

3.4.8.2 LM317MDT-TR

The LM317MDT-TR is another alternative to an adjustable output linear voltage regulator. This component comes in a smaller package with an even smaller set of pins. Its functionality, however, is still based on several components such as resistor ratios and by-pass capacitors. In contrast to the MAX25302BATD/V+, it has a different equation to solve for the desired voltage output as well as a different typical application schematic as the datasheet shows.

Equation 1

$V_0 = V_{REF} (1 + R_2 / R_1) + I_{ADJ} R_2$

For this calculation we do not have to use the element of Voltage feedback, however, we have the current of the adjustable pin plays a slight role and deals a variation that is minimal, but present, in the voltage output. The maximum value of I_{ADJ} is 100uA which may influence the output voltage by a tenth of a decimal depending on the resistors chosen.



Figure 21 - Typical Application of LM317MDT-TR per Datasheet

In conclusion, for voltage regulators, we believed it was best to choose adjustable linear voltage regulators based on their focus on being low noise since we are dealing with many optical sensitive components as well as the ways output can be manipulated easily.

From these components the best choice for our project would be the LM317MDT-TR, and this is for the simplicity of the component, small size it requires within the PCB, and because of the shapes and sizes of pads being best for our undergrad design.

3.4.8.3 TPS563300DRLR

The TPS563300DRLR is a synchronous buck converter designed by Texas Instruments. This efficient non-linear voltage regulator is specifically designed to convert a higher input voltage to a lower regulated output voltage by stepping down the first within its internal circuit, making it a key component in power management and distribution system of our project.

The key features of the TPS563300DRLR start with an input voltage range of 3.8V to 28V, accommodating a wide range of power sources which was desirable for us since we were in a space of limbo between choosing a main power supply unit of either 12V or 24V and this buck converter could fit both options.

The output voltage range is 0.8V to 22V, which is adjustable via an external resistor divider which is shown in Figure 15 from the design of TI webench on how the voltage divider is put in place.



Figure 22 - Imported schematic from TI webench on TPS563300 for 3.3V.

The output current capacity is up to 3A, it is suitable for powering a variety of loads, our main power supply will have 5A and 3A will be more than overkill to power up the components on the side of the circuit the regulated power will be going into. The converter also offers high efficiency, that is up to 95%.

Overcurrent and thermal protection are also provided to safeguard the converter and the connected load from potential damage which is a desirable feature as it can make the overall designing of the circuit much simpler. The converter also operates at a switching frequency of up to 500 kHz, that enables the use of small external components, such as inductors and capacitors, which results in a compact, space-saving design that we got from TI webench as it is seen once again in the above figure. The TPS563300DRLR is versatile and can be utilized in numerous systems and applications that require precise voltage regulation and efficient power management. Typical use cases include industrial and automation systems, where the converter can power microcontrollers, sensors, actuators, and other digital or analog loads.

The design shown will be used to power up the microcontroller, circuit-side isolation of the USB input for the microcontroller, as well as the temperature and humidity sensor as these three require a voltage input of 3.3V and it will be up to standard on the current it can deliver based on specifications.

TPS563300DRLR will also be used for the 12V rail capable of delivering 3A. This rail's function will be to power the DC fan to deal with humidity and temperature. In Figure 16 below we can see how the inductor and adjusting resistors are modified to use the same buck converter component while generating a different output voltage as it is needed for the correct functioning of the project.



Figure 23 - Imported schematic of the 12V rail circuit by TPS563300DRLR.

We can see the difference from R1 and R5 as they are 30.9k and 140k respectively. Resistor R6 remains 10k due to manufacturer's specifications for the best functioning of the device at use in the circuit. The following equation gives light to the reasoning behind the values of these resistors.

$$\mathsf{R}_{\mathsf{FBT}} = \frac{\mathsf{V}_{\mathsf{OUT}} - \mathsf{V}_{\mathsf{REF}}}{\mathsf{V}_{\mathsf{REF}}} \times \mathsf{R}_{\mathsf{FBB}}$$

Where $R_{FBB} = R6 = R2 = 10$ kOhm and it is to remain unchanged through different set ups, and $V_{REF} = 0.8$ V. For each rail that we desire, in our case, 12V and 3V3 which is schematic practice for 3.3V, we input the voltage values into Vout and solve for the remaining resistor R_{FBT} which would give us the values of 30.9k and 140k ohms for our different rails.

In the following table, we have been explaining how every one of the different voltage regulators would contribute to our design and the reason the buck converter was chosen as well as the different characteristics of the components.

The main reason, however, was the simplicity of being able to use TI webench to complete the design and have a reliable guideline portraying the use of different capacitors and inductors along with their respective values.

Feature	TPS563300DRLR	LM317MDT-TR	MAX25302BATD/ V+
Voltage Rating	3.8V – 28V	4.2V – 40V	1.7V – 5.5V
Current Drawn	20 uA	-	1.3mA
Max Current Output	3A	1.5 A	2A
Voltage output	800 mV to 22 V	1.2 V to 37 V	600 mV to 5 V
Size	1.6-mm × 2.1-mm	2.4mm x 6mm	SOIC-8
Pins	8	4	14
Price	\$1.70	\$0.90	\$1.94
Reasoning	Buck converter, TI webench simplicity	Outdated component	TDFN package, Does not meet new output requirements

Table 11 - Converter options and characteristics

As described in the reasoning row, the TPS563300DRLR was chosen for being a buck converter which offers great reliability as well as the opportunity of importing a design from TI webench.

The LM317 seemed like a great option but after some investigation and second opinions we decided that the component was too outdated for our design and would rather pick somewhere else with more functionality and reliability.

The linear voltage regulator MAX25302 seemed like the perfect fit as it is a newer component with a lot of functionality that met our specifications at first as we were only looking to need a rail of 3.3V before we changed our power unit supply to one providing 24V which meant we now needed a 12V rail. Regardless, the component is shown as a TDFN package which is not an attractive feature for us since it would make testing and troubleshooting harder in both PCB and breadboard.

3.4.9 Pad Shaping & Sizing

The size of pads and shapes has a critical role in the way we have choose the parts for the printed circuit board. The importance of pad shaping and sizing will be a major factor for us in the topics of manufacturability, troubleshooting and avoiding failure. On that note, ideal pad design is essential for visual inspection and testing purposes. Adequate pad sizes and outside-showing shapes allow for easier inspection of solder joints and make it much more convenient to probe and test individual components, communications, and connections on the printed circuit board. Furthermore, it makes it easier to remove and replace components during rework or repair, minimizing the risk of damage to the printed circuit board or other components. Since soldering, and troubleshooting a PCB overall, is a factor that will be new to us as undergraduate electrical engineers, pad sizes and shapes in a manner that reduce the risks of damaging a time critical board and components that also cost us money, is a big factor in deciding what parts to pick.

3.4.10 Safety Interlocks

Safety interlocks are special safety tools that disallow operation of machinery if there is danger to the operator. They are installed to ensure the safety of everyone around them. The job of this device is simple but extremely important. It is responsible for keeping the spectroscope sealed of any laser beams leaking during the scanning.

This was a feature added at the request of our sponsors, Ocean Insight. They knew there could be some problems if someone carelessly opened the hatch so they requested that the safety interlock not only locked the door, but if someone was somehow successful in opening the door while the laser was active, the laser would immediately shut off. This mechanism will be enabled by the sensor on the latch that detects when the door is opened or closed. By using this signal, we have been able to use a simple PCB that waits for that signal to arrive. If the signal arrives, the voltage will increase in the board which will send a signal to the laser to turn off. Ideally, this will never happen as the door itself is already locked and cannot be opened but "if there's a will, there's a way" and we want to ensure the safety of everyone is guaranteed when operating our spectrometer.

The principle of a safety interlock is simple, inside the safety interlock we have a normally open or normally closed contact. This contact is the one that energizes the coil inside the switch to change the contact from open to closed and back. For a normally open switch, energizing the coil will cause the switch to move and then the circuit becomes closed, allowing current to flow. For a normally closed switch the opposite is true, the circuit is closed allowing current to flow. When the coil is energized, the switch will move to the open position, cutting the current from the circuit. Alongside monitoring circuits built into the safety interlocks, which allow us to also know if the interlock is engaged or not. These monitoring circuits are also necessary since the main circuit only operates the safety interlock and does not send information on whether safety interlock is engaged or not. Finally, we have the actuator, which can be considered a key of sorts. The actuator is a metal piece attached to the sliding window in our case. When the sliding window is closed the actuator goes into the safety interlock. This should engage our monitoring circuit that the window is closed, and that the actuator is in position to be engaged. A separate monitoring circuit allows us to know whether the actuator is engaged or not. Once both of our circuits are given the ok, then we allow the laser operations to begin.

3.4.10.1 Banner Engineering SI-LS42DMMGF

The Banner Engineering is an electronically operated mechanical lock that is normally used for industrial purposes. However, for our purposes this will work fine. It will lock the door under circumstances you program it to and will release the lock again under the circumstances you program it to do so. One problem that can be seen with it is the lack of mounting mechanisms, this might lead to new mounting mechanisms being introduced, such as drilling new holes into our enclosure. Making holes into our enclosure that is not already there is a difficult thing to do. Given the fact that we have been using to be using a laser inside our enclosure, drilling holes into it will also lead to leakage of our electromagnetic radiation. The power levels at which we have be operating at will cause these beams to leak and cause harm or serious injuries to people, which is the exact opposite of what the safety interlock is supposed to do. The safety interlock also comes with options for normally closed and normally open contacts that operate it.

3.4.10.2 IDEC HS1L

The HS1L, made by IDEC, is another interlock that caught our eyes. It allows for mechanically locking our enclosure while scanning with the usage of NO/NC terminals in the interlock. It has 4 possible states with 3 of them denying machine operation until safety is properly reinstated. The HS1L also has a 24V coil for the solenoid lock built in. This means that it can work with the power supplies that we have looked at, meaning we can power the safety systems without needing a separate circuit. The way that it will work is using a relay, much like Arduino boards use. The difference is that we have integrate the relay ourselves into our PCB alongside our microcontroller to satisfy the PCB design aspect of senior design. An additional feature of this safety interlock is the door monitor and lock monitor circuits built into the design, this allows us to read the status of the lock and the actuator. If the actuator is activated but the lock is not, then we know that the door is closed but not locked. If both are activated, then we know it is locked. This can ensure proper backup in case the actuator fails to lock, and we can warn the user about this if we so choose to implement this feature. The actuator itself is sold separately, so we have need to buy it as alongside the safety interlock. This is great because IDEC sells multiple actuators for this specific model, therefore we have guaranteed compatibility.

3.4.10.3 Omron Automation and Safety TL4019

The TL4019 is another interlock that caught our eyes, it has all the features we need and some additional extras. Controlled through a normally closed logic, like all the other interlocks we have. It also has a lock circuit and door monitor circuit like the IDEC HS1L, which is great since we get to monitor the lock and monitor the door in this case as well. The TL4019 also has 8 different actuator positions for entry so we can make it fit in most circumstances. Furthermore, it is smaller than the IDEC HS1I and the same size as the Banner engineering SI-LS42DMMGF, which would make it compatible with the as a replacement part in case the SI-LS42DMMGF breaks or is unsuitable to our needs. The option of using different actuators for this model of safety lock is also appealing. Being able to adjust our enclosure to fit different types of lock could allow us to implement more safety interlocks in the future, should regulations and design standards require this. Manual release latches on the interlock are a safety issue but given that the safety interlocks will be in the enclosure itself this is a negligible point. If someone can use the manual interlock release, then that means the enclosure was already breached to begin with.

	Banner Engineering SI- LS42DMMGF	IDEC HS1L	Omron Automation and Safety TL4019
Max Holding Force (Locked)	1500N	3000N	1200N
Operating Temperature Range	-20C to 70C	-20C to 55C	
Power Consumption	4.4W	4.8W	8W
Operating Voltage	110/230VAC or 24VAC/VDC	24VDC	24VAC/24VDC Or 110VAC
Switch Operations per hour.	600	900	
Maximum Actuator Speed	0.5m/s	1m/s	0.33m/s
Mechanical Life operations	1000000	1000000	1000000
Price	~426\$	~200\$	~552\$

Table 12 - Automation and safety performance characteristics and key parameters tabulated.

After comparing our various safety interlocks, one of them stands out as the clear winner, the IDEC HS1L. This interlock features the highest locking force out of all of them at 3000 Newtons. This is the equivalent of lifting 300 kilograms of weight which would be almost impossible for the average human to do, this would lead to breaking our enclosure before breaking the safety interlocks. The other interlocks on this list listed lower maximum force ratings and for that reason they are disqualified. 1500 Newtons and 1200 Newtons of force may sound like a lot, but if the average person put their entire weight behind opening the door to our
enclosure, they would be able to break the safety interlock, exactly the type of situation that our safety interlocks are being designed to avoid. Other reasons that the IDEC HS1L stands out among the other is the switch operations per hour, at 900 operations per hour we can operate the safety interlock every 4 seconds. This time is more than enough for the safety interlock to be ready for the next operation. Scanning 100 samples with our spectroscope is going to take some time. Price is also a consideration in this case, being twice as cheap as the other options on the list. The operating temperature of the device is not of concern for us, given that we have not be operating this at temperatures higher than 55C. Having the highest actuator speeds is also great since moving the sliding window on our enclosure is generally done quickly. With these facts in hand, we have decided that the IDEC HS1L is the best option for our use case scenario.

<u>3.4.11 DC Fan</u>

When dealing with temperature and humidity a great way to account for this factor is to implement a DC fan. A DC fan is an essential component for maintaining thermal and humidity stability within a printed circuit board and its external components. Proper heat dissipation has become critical to ensure the reliable performance and longevity of the components as electronic devices become more complex and their power densities increase especially such powerful devices like processors and lasers that we have implemented into our design. DC fans aid by actively circulating air around the PCB, which dissipates the heat, dries out the environment and prevents overheating as well as a proper environment for the electronics components.

When considering a DC fan for a PCB, the most important characteristics we looked at were airflow, noise level, speed, voltage, power consumption, size, connector type and current drawn. Airflow, which is measured in Cubic Feet per Minute (CFM), represents the volume of air a fan can move in each time. Greater CFM values showcase a fan's ability to move more air and provide better cooling performance. Choose a fan with sufficient airflow to cool your specific PCB and components based on their heat generation and thermal requirements.

The noise level is represented in dBA (decibels A-weighted) and indicates the noise generated by the fan during operation. Lower dBA values indicate quieter fans. Our fan selection will be based on the best balance of dBA and CFM as we want great airflow at the time as not such a noisy environment within the device. Through research we have found that 30-40 dBA would be optimal for a quiet operation of the fan and overall functionality.

Speed is measured in Revolutions Per Minute (RPM), it indicates how fast the fan blades rotate. The higher the RPM values are the higher the airflow and better

cooling performance. In this sense, RPM is directly proportional with both dBA and CFM. The DC fans we have be looking at come in voltage ratings of 12V and 24V.

The size is also a great characteristic to keep in mind the fans we are selecting come in sizes of 40x40mm, 60x60mm, 80x80mm, and 120x120mm. We are not expecting our PCB to be of great size so the 80x80mm we believe would be optimal for a DC fan. These fans come with a different number of cables that serve different functionalities such as PWM signal, tachometer signal and the regular voltage and ground supplies. The PWM signal would come from a designated circuit that controls the RPM of the fan. The tachometer is an output signal that would be read and would show the proper functioning of the DC fan.

3.4.11.1 CFM-8015BF-130-301

After careful examination of the many features and exploring the datasheet publicly posted by CUI DEVICES on the DC fans family of CFM-80BF we have decided to select the CFM-8015BF-130-301 as our fan to support the humidity and temperature factors within our PCB and the external components.

This DC fan component comes with a voltage rating of 10.8-13.2V for which we have be providing 12V coming from the buck converter circuit derived from the 24V power supply unit. The fan draws a current of 0.26mA being the main reason a lot of the fan circuit logic components were picked out as driving a current that may not seem high, but is, may be a complex task when dealing with logic.

The RPM for this device comes at 3,000 which is a good number as it falls right in the middle of the value ranges for this characteristic. The dBA and CFM are 30.1 and 34.65 respectively which after the research in the meaning behind the values and comparing them with other technologies are in a very good spot of the specifications as we desire them. It comes with 2-wire connectors only needing a voltage of 12V and the corresponding ground supply. The simplicity of the wiring is the most important characteristic for picking this component.

<u>3.4.12 Relays</u>

Relays are commonly used electronic devices that provide us with an electronically controlled switch. They come in many forms and sizes ranging from high to low voltage and can be controlled with a small amount of current. Relays are basically switches that allow us to control higher voltage levels with lower voltage levels. The relay has an induction coil inside that gets magnetized. Once magnetized, this coil flips the switch inside the relay itself. Once this switch is activated, power flows through the circuit, or power is cut off from the circuit. Normally open relays, as the name would suggest, are in an open circuit state by default. Once the coil is energized the switch moves to the closed position and power flows through. Normally closed relays are the opposite, closed circuit by default, and then open

circuited once the coil is energized. The normally closed relay is usually used in safety systems where you must detect something. For example, a sensor detects a gas leak in a turbine, and the normally closed relay is activated to cut power to the pumps to avoid danger. Normally open relays are basically on/off switches. It is important to note that most relays offer both positions in the form of having 3 contacts. These contacts are normally closed, normally open, and common. Connect a wire to common, and another one to the normally open or closed position for the desired operation. In our case we are looking for a simple normally open relay. That way the default position for our safety interlocks is off. This means that we won't be locked out of our device in the case of the power going out. The relay itself needs to be able to be controlled by our microcontroller and so we need to be able to activate it with 3.3 Volts DC. The problem with this is that our microcontroller is not able to source enough current for this. The solution is simple, we use a relay alongside a transistor to boost the output current of our microcontroller so that we can use the GPIO pins on our microcontroller to effectively control the safety interlocks. The coil voltage of the relay is an important parameter to consider. Relay coils can generally be operated by different voltages. We have been using to be using a relay with a 3.3 Volt DC coil, this will allow us to have the same voltage level for the relay as the microcontroller and most of our peripherals. We also need to make sure that the contacts on our relay can handle the current that the safety interlocks will be drawing. This is important for both constant current and peak current. Operating temperature range is also a consideration for this part, since it will be located alongside other equipment that produce heat in a small environment.

3.4.12.1 CUI Devices SR5-3V-200-1C

This relay has a coil voltage of 3 Volts DC. Although it is slightly different than the 3.3 Volts DC supplied by the GPIO pins. The specifications sheet allows for a slight deviation of input voltage. The coil type is non latching as well, it does not retain its state when powered on and off. This is a good thing in this case, because once we power off our systems, the lasers will no longer be operational. And the danger is gone, therefore there is no reason to have a latching relay. Another bonus of this relay is that is a type C relay. Type C relays allow us to choose whether relay operates in a normally closed or normally open manner. Type A relays are only normally open, and type B relays are normally closed.

The mounting system leaves a bit to be desired though, since it used through hole pins instead of the more common SMT mounts, this is not a negative trait in and of itself. Having components that all use the same mounting mechanism is simply a good way to streamline production.

3.4.12.2 Omron Electronics GV5-1-DC3

The GV5-1-DC3 by Omron electronics is another relay that we have be looking at for our purposes. This relay also uses through hole soldering pins as its mounting

system, which again introduces different mounting systems into our design. It is a single pole double throw design. This means that it has two poles with a single throw. In other words, it can be used as a normally open or normally closed relay depending on how you wire it. This gives more flexibility in our design.

3.4.12.3 TE Connectivity 5-1462037-5

This relay by TE connectivity also checks most of our boxes. The coil is operated at 3 Volts DC. Unlike the other two relays, these ones use standard SMD/SMT mounting mechanisms like most of our other components. One issue with this is that it is a latching relay. The latching relay will stay in its position even when powered off. This is an issue since when powering off the entire device, we expect to be able to open it. But if we were to power it off without making sure that it is unlocked, we would have to power it on again to remove the lock. We can always open the enclosure to reach it, but customers would not want to. One thing this relay does have compared to the others, is a double pole double throw design. This relay includes a normally open circuit, and a normally closed circuit. This design gives us more option to control the safety relay circuit by changing the voltage polarity at the relay contacts. This can be useful for things such as DC motors where you only want forward and reverse functions. However, the coil on our safety interlock has no polarity, therefore we have no need for changing the polarity on the power source, it is however a nice feature to have.

		Omron	TE Connectivity
	SR5-3V-200-1C	Electronics GV5- 1-DC3	5-1462037-5
Coil Voltage	3VDC	3VDC	3VDC
Coil type	Non-latching	Non-latching	Latching
Coil Current	66.6mA	50mA	33.3mA
Contact current rating	1A	1A	2A
Coil Resistance	450hms	60Ohms	90Ohms
Туре	SPDT	SPDT	DPDT
Power Consumption	200mW	150mW	100mW
Price	~1\$	~2\$	~1\$

3.4.12.4 Comparison of relays

Table 13 - Tabulation of relays compared.

Right off the bat we can see that price is not really a constraint when it comes to picking which relay, we have been using. The safety interlock that we ended up

picking has a maximum current of 200mA when in use, so the current ratings of all these relays are well within spec of the current requirements. One relay that we have not be using is the latching relay from TE connectivity, although it offers the lowest power consumption, the difference is negligible in this case, and it does not offset the latching nature of the relay. Coil resistance is negligible in this case as well. This leaves us with two relays to choose from. Since our 3.3 Volt DC is being provided by our power supply that is built onto the board, we want to reduce the current draw on it as much as possible to give ourselves more headroom to work with. The CUI devices relay uses more power and has a higher coil current usage than the one offered by Omron electronics. Since both relays are single pole double throw, this becomes the deciding factor for our design.

4.0 Optical Design

This section of the paper will discuss mathematical equations and simulations. It will show how the project components optically were chosen and how they will be the best for our project design. The equations will include important aspects of our project that need to be stable for our basic specifications for the project to be met. For the simulation of the equations and the optical design we used ZEMAX and MATLAB to show the prototype of the setup.

An optical design is important to the whole project being successful because the project is mainly optically focused. By using those optic equation, it can be useful in ensuring that our optical design works as intended. By using MATLAB, you can perform complex calculation and simulations to test different scenarios and optimize our design parameters. Which we have done in certain cases to with the components that will be talked about in the sections below. ZEMAX is an optical design software that allows the us to create, test and analyze our optical system before it is built. With that using optics equations can help us better understand the physical principles behind what we want to do before using simulations.

4.3 Optical Components

The optical components will be discussed below on how they parts were selected for this project. The components will need to be carefully picked out to get the desired results we want from this project. However, since we are sponsored some of the optical components were given to us and we had to work around the design specification for those parts. When certain things were given to use, we must make sure that it would not deter of from getting the final experimental results we expect to see.

4.3.1 Diffraction Gratings

The diffraction grating was chosen based on what was accessible in the market and what would give us a good spectral range. Choosing a groove density of 300 lines/mm would results in a great resolution. This means that the spectrometer would be able to distinguish different wavelengths that fall within the spectral range.

This groove density would be reasonable with to light dispersion and how it will be collected by the detector. This is important because it will be collected by the defector that affects the signal-to-noise ratio to the spectrometer. A groove density of 15 grooves/mm was also debated to be inputted into the optical design, but we wanted to have a good resolution, so the 300 lines/mm was shown to be the best solution.

The diffraction grating that was chosen has a 300 grooves/mm, with a blaze wavelength 760 nm and had dimension of 12.5mm. The groove density of a diffraction grating is defined as the number of grooves per unit length on the length on the surface grating, $N = d^{-1}$.

The Littrow angle is an important feature in why the spatial heterodyne spectrometer is advantageous because it allows for efficient coupling of light into the spectrometer, and it also allows to use a smaller instrument. In an SHS, the angle at which the incident light is diffracted back along its path of incidence.



Figure 24 - Diffraction Grating (Littrow)

Diffraction Grating	Edmund Optics (Richardson Grating)	Edmund Optics (Richardson Grating)	Thorlabs (GTU13-03)
Groove Density (grooves/mm)	300	150	300
Blaze Wavelength (nm)	760	300	235
Length x Width (mm)	12.5 x 12.5	12.5 x 12.5	12.5 x 12.5
Peak Efficiency (%)	79	61	-

Table 14 - Grating properties including groove density, blaze wavelength, size, and efficiency.

The table above shows the different gratings the optical team was looking into so that the spatial heterodyne spectrometer would work. The grating that was chosen was the Edmund Optics 300 groove density to be fit out project. Even when switching to a 532 nm laser we still used the same grating because of our time constraints but we were still able to get results from the part that we have selected.

4.3.2 Lenses

Below is a coating curve showing the reflection vs wavelength efficiency of the lens that we plan to use to image the interference fringes onto the detector. Note that this lens has reasonable transmission within the designed spectral range of our system. This lens has an effective focal length of 10mm at 780nm. This lens will can be changed depending on the where we place the detector.



Figure 25 - Coating curve for NIR Aspheric lens used for imaging the interference fringes of the SHS.

Our design also includes a fiber collimator as well as a beam expander to help ensure the light is not diverging and properly fills the size of our optics in our system.

4.3.2.1 Imaging Lens

The imaging lens has been a challenging par in the project to be able to implement in the design. To determine the focal length of the imaging system, I have used the thin lens equation. In this case, the object distance is infinity since the rays are coming from infinity from the spectrometer. The image distance is the distance at where the CCD camera is because that is where the detection of the fringes will be looked upon. The distance that I measured was about 2 inches away. Which is 50.8 millimeters. The imaging lens equation is:

$$\frac{1}{f} = \frac{1}{d}$$

With that equation the focal length would simplify to:

$$\frac{1}{f} = \frac{1}{50.8 \ mm}$$

The focal length would be f = 50.8 mm. Therefore, the focal length of the imaging lens should be approximately 50.8 mm to image the infinity rays from the spectrometer onto a detector.

Looking for these specifications on the internet was a bit challenging to investigate. The imaging system can always be moved depending on where the detector is on the breadboard. We might have to get our project manufactured because most of the lenses that we have seen doesn't really fit our specifications, but we can always modify the imaging part to the lens that we have picked.



Figure 26 is the Keplerian imaging set-up that the team was going to use before modifying the set up at the end of the semester in Senior Design 2.

For a Raman spectrometer to effectively analyze water, a suitable imaging system is necessary because it has a significant impact on the instrument's overall performance. The excitation laser is focused onto the sample by the imaging equipment, and the Raman signal produced by the laser-sample interaction is then captured. The sensitivity, resolution, and accuracy of the Raman measurement can be significantly impacted by the caliber of the imaging equipment.

Due to its high refractive index and significant Raman scattering, water presents a difficult sample for Raman spectroscopy. As the excitation laser beam passes through the sample, the high refractive index of water can create considerable distortions that diminish the signal strength and increase noise in the Raman measurement. Additionally, the considerable fluorescence background that can result from the water's strong Raman scattering can obstruct the ability to identify the Raman signal.

An update about the Keplerian lenses. We did not incorporate them into our project because it was not going to be effective in getting the images from the grating to the detector.

4.3.3 Optical Cage Components

The optical cage components consist of metric to imperial adaptors to secure the cage plates to the breadboard, which consists of 8 holes separated by inches vertically and horizontally. We are using a variety of components from Thorlabs to fit a 16mm cage system, the system required to house half inch optics.

We've also collaborated with Ocean Insight to develop a custom grating mount. This grating mount is designed to house the grating at the Littrow angle after simply sliding the grating in. This mount also comes with adjustable tip and tilt controls for fine tuning of grating angle. There are also a variety of cage plates and kinematic lens mounts that will slide along the rails of the cage system.

4.3.4 Fiber Collimator

Fiber collimation is an aspect of Raman spectroscopy, as it ensures that the laser beam exiting the fiber is properly focused onto the sample and that the Raman scattered light returning to the fiber is efficiently collected and directed to the detector. One way to achieve fiber collimation is to use a lens or lens system to focus the light from the fiber into a collimation beam. A fiber collimator, which is a specialized device designed to collimate the light exiting the fiber, is another approach for accomplishing fiber collimation. A fiber collimator is typically made from a lens or lens system installed in a housing designed to be attached directly to the fiber. After that, the collimated beam can be directed to the sample, and the Raman scattered light can be collected and guided back into the fiber.

In any instance, it is critical to ensure that the collimated beam is appropriately aligned with the sample and that the system's collection efficiency is optimum for Raman scattering. This can be accomplished through careful lens or lens system adjustment, as well as the use of specialized optics, such as filters or polarizers, to maximize the Raman spectrum's signal-to-noise ratio.

Overall, fiber collimation is a crucial feature of Raman spectroscopy since it helps to assure high-quality data and correct sample analysis.

4.4 MATLAB Calculations

We used MATLAB to perform calculations. We found this to be a convenient tool to perform multiple calculations in one go after changing a few fundamental parameters, namely optics size and excitation wavelength. We knew we wanted optics that were ½ inch in size to favor a more compact design.

A lot of our design was inspired by the detector that our team was already in possession of. The detector has 1944 pixels horizontally. This number is important to determine the overall spectral range our spectrometer can have, and the spectral range depends on the resolving power.

By fixing the optics size and number of pixels, we chose to focus on groove density and excitation wavelength. We found the best wavelength to use would be 532 nm as this would still have fluorescence but enable us to achieve a larger spectral range. Choosing this wavelength then implies we need optics that are efficient in the visible and near infrared region of the electromagnetic spectrum.

The optics size is set to 12.7mm, the groove density is set to 300 grooves/mm. The next set of lines of code would be responsible for the calculations. First the resolving power is calculated. Once this is calculated, the spectral range can be determined.

After the spectral range is determined, then the band is determined. The Littrow angle can be determined at any point in the code. The FWHM can be calculated once the resolving power is known. In the below image, an example of a few lines of code can be used to determine the Raman signal wavelength:

%Desired Raman Shift in cm^-1
ramanShift = 3500.
ramanWL = 10^7/(10^7/(excitationWavelength)-ramanShift); %EW is set to nm
Figure 07. Evenuels of ande to calculate the Demon signal wavelength

Figure 27 - Example of code to calculate the Raman signal wavelength.

The purpose of the section is not to show the code itself, but to share the underlying approach behind the calculations. Resolving power is a key parameter to calculate, and there are a variety of fixed constants to be used throughout the calculations which will be described in further detail in the Spectrometer design section of this report. You can see the result of these calculations based on a screenshot of the MATLAB workspace in figure 26.

Name 📥	Value			
🚽 band	[785,884.7218]			
🛨 dWL	1.6718			
🛨 excitationWaveleng	785			
FWHM	0.1030			
🛨 grooveDensity	300			
littrowAngle	6.7623			
N	1936			
🛨 ramanShift	3500			
🛨 ramanWL	1.0824e+03			
🛨 resolvingPower	7620			
🕂 spectralRange	99.7218			
widthOfOptics	12.7000			

Figure 28 - MATLAB workspace containing results of calculation.

As seen in figure 22, choosing our laser wavelength and Littrow wavelength as 532nm, and optics size of 12.5mm, using a detector with 1944 pixels across the array, and using gratings with 300 lines/mm:

$$FWHM = \frac{\lambda_{Laser}}{Resolving Power} 0.1030nm$$

$$\delta\omega = Raman \ resolution = 10^7 \frac{FWHM}{\lambda_{Laser}} \lambda = 1.67 cm^{-1}$$

$$Resolving \ power = 7620$$

$$Spectral \ Range = N \frac{\lambda_{Laser}}{2 * Resolving Power} = [532, \sim 600] = 68nm$$

$$Raman \ Signal \ Wavelength = 2130 \ nm \ (Raman \ Shift \ of \ Water = 3500 cm^{-1})$$

Note that this system would not be able to detect the Raman signal of water as 3500nm is outside of the range that our spectrometer is capable of detecting. However, it would be able to detect a sample of Sulfur whose frequency shift would produce a Raman signal within our spectral range.

The theoretical value of our spectrometer's resolution is 0.1030nm in terms of wavelength. In terms of wavenumbers, the resolution is $\delta \omega = 1.67 cm^{-1}$, which is far smaller than the expected $20 cm^{-1}$ from our requirement specifications. Again, this is an ideal theoretical value for resolution.

It should be emphasized that we are attempting to use smaller sized optics to make the spectrometer compact and that we are using an excitation wavelength of 532nm to promote a larger spectral range. All of this, including grating groove density, helps to achieve a higher resolution.

4.5 Spectrometer Design in ZEMAX

The Spatial Heterodyne Spectrometer as previously mentioned is a static interferometric Fourier transform spectrometer. Interference fringe patterns are generated and imaged upon the detector. Our group has chosen ZEMAX as the tool we shall use to model the device.

ZEMAX has two modes used in optical design, sequential and non-sequential. Sequential is useful for optical designs and can be used for a variety of purposes such as aberration correction or general optical design.

However, in this mode, rays are traced from point to point in sequence. It is difficult to generate a design of an interferometric spectrometer in this mode. Despite this, ZEMAX offers optical design in non-sequential mode. This mode is particularly useful for designs that require the analysis of an optical system in which ray analysis can be extended from beyond point-to-point analysis.

Stray light reflecting off surfaces or the interference of rays can be analyzed in this mode. Rays can travel in one direction and then redirected along that path of propagation and reflect off another surface in the design as opposed to traveling from point A to point B.

Nonsequential ray tracing doesn't rely on a predefined sequence of surfaces in which rays strike. This is useful for generating interferences fringes.



Figure 29 - Michelson Interferometer Developed in ZEMAX

In our approach to designing the spatial heterodyne spectrometer, we first attempted to model the Michelson interferometer to become more familiarized with developing optical systems in non-sequential mode. See *figure 24* on the previous page. As mentioned previously, the Michelson interferometer involves taking a beam of light, splitting it into two separate beams via a beam splitter and then recombines them. The optical path length difference between the two arms of the interferometer determines the interference fringes that are imaged upon the detector.

	Object Type	Col	Rei	Ins	X Positior	Y Positior	Z Positior	Tilt About)	Tilt About 1	Tilt About 2	Material	X Half W	Y Half Wi
1	Source Rectangle*		0	0	0.000	0.000	0.000	0.000	0.000	0.000	-	10	3.5E+05
2	Polygon Object 🔻	sp	0	0	0.000	0.000	10.000	45.000	0.000	0.000	BK7	4.000	1
3	Rectangle 🔻		0	0	0.000	0.000	20.000	0.000	0.000	0.000	MIRROR	4.000	1.000
4	Rectangle 🔻		0	0	0.000	8.000	10.000	90.000	1.000	0.000	MIRROR	4.000	1.000
5	Detector Rectang	i	0	0	0.000	-10.000	10.000	90.000	0.000	0.000	ABSORB	1.000	1.000

Figure 30 - non-sequential component editor in ZEMAX for the Michelson interferometer design

In the figure above, you can see how we approached the design of the Michelson interferometer. This is a view of the non-sequential component editor. In our design of the Michelson interferometer, instead of changing the physical distances of the mirrors from the beam splitter to adjust the optical path length difference, we chose to generate fringes by adjusting the tilt of the system about the Y axis. This seemed to be sufficient in generating the interference pattern. See the figure below.



Figure 31 - Detector viewer of the Michelson Interferometer using a show data of coherent irradiance and displayed as an inverse gray scale.

Once the Michelson interferometer was developed in ZEMAX to produce *interference fringes in general*, we moved forward to design the SHS via the physical parameters set by the optical breadboard that we had chosen while adhering to the project requirements specifications. With about 8 inches by 8 inches of working space, we needed to ensure that we accurately modeled the physical distances in which the optics were separated.

As the SHS is basically a Michelson interferometer with diffraction gratings instead of mirrors in place, we had to make minor non-sequential component adjustments.

	Object Type	Co	Rei	Ins	X F	Y Position	Z Position	Tilt About X	Tilt About Y	Tilt About Z	Material	# Layout Rays	# Analysis Rays
1	Source Rectangle -		0	0	0.0.	0.000	0.000	0.000	0.000	0.000	-	1	5E+05
2	Polygon Object 🔻	sp	0	0	0.0.	0.000	80.000	45.000	0.000	0.000	BK7	12.500	1
3	Diffraction Grating •		0	0	0.0.	80.000	80.000	-96.762	0.000	0.000	MIRROR	0.000	0.000
4	Diffraction Grating •		0	0	0.0.	0.000	160.000	6.762	0.000	0.000	MIRROR	0.000	0.000
5	Detector Rectangle 🔻		0	0	0.0.	-40.000	80.000	90.000	0.000 V	0.000	ABSORB	3.000	3.000
	Object Type	Clear	1		Edg	ge 1 1	hickness	Radius 2	Conic 2	Clea	ar 2	Edge 2	Lines/µm
1	Source Rectangle •	1.0	000			0	0	0.800	0.800	D	0.000	0.000	0.000
2	Polygon Object 🔻												
3	Diffraction Grating •	12.5	500		1.	2.500	1.000	0.000	0.000	0 1	2.500	12.500	0.300
4	Diffraction Grating •	12.5	500		12	2.500	1.000	0.000	0.000	D 1	2.500	12.500	0.300
5	Detector Rectangle •	5	500			500	0	1	1	1	0	0.000	0

Figure 32 - non-sequential component editor for the SHS

To configure the gratings, we set the groove density to 0.3 lines/ μm (300 lines/nm). The gratings were also configured to have a Lambertian scatter model to simplify

the wavefront analysis by modeling a perfect diffuse surface that scatters light equally in all directions. We also set the gratings to diffract only the ± 1 and 0 orders.

 ∧ Object 3 Properties < > 								
Type Draw	Split:	Split by table be	low	~				
Sources	DLL:	diff_samp_1.DLL		÷.				
Coat/Scatter Scatter To	Start Order:	-1	Stop Order:	1				
Volume Physics		Reflect:	Copy ->1	Transmit:				
Index	Order -1:	0.99	Order -1:	0				
CAD	Order 0:	0.99	Order 0:	0				
	Order 1:	0.99	Order 1:	0				

Figure 33 - Object 3 (and 4) diffraction properties

Our optics in this model are all set to the $\frac{1}{2}$ inch size. This is consistent with the previous calculations in our SHS design. The first diffraction grating (object 3) is set to an angle of $90^{\circ} + 6.762^{\circ}$ to achieve the Littrow configuration where the first diffracted order is returned along the incident path of propagation. The second diffraction grating is set to the Littrow angle itself ($\theta_L = 6.762^{\circ}$). To use the diffraction gratings as reflective, the material type is set to MIRROR. The beam splitter is simply set to 45° . This is the default beam splitter model under the polygon objects that Zemax offers.

The gratings are both *equidistant* from the beam splitter by about 80mm or \sim 3 inches. Keep in mind that one of the advantages of this type of spectrometer is that this spectrometer can be made more compact as long as various parameters such as optical size, blaze wavelength, Littrow wavelength and angle are kept consistent, but importantly, that the gratings are equidistant from the beam splitter.

Just one wavelength set to 532nm with a single layout ray was used to "align" the SHS as seen in the figure on the next page.



Figure 34 - NSC Layout of the SHS

In the figure above, the first diffracted order is redirected back towards the beam splitter. The other diffracted orders are cut off as there is, based on the size of the system, no surface for those rays to strike. In the actual device, there may be a wall in which these rays may scatter from, so placement of baffles to absorb the scattered light may be considered.



Figure 35 - NSC Shaded 3D Model of the SHS using 1000 layout rays with a variety of wavelengths.

The resulting interference fringes of the system is seen in the figure below. Note that the view is rotated by 90° since optics are rotated around the *x*-axis of the system and the placement of the gratings are along the y-direction while rays propagate forward through the z-direction.

The detector view has the y-direction set vertically and the x-direction along the horizontal. In the actual system, the fringes will vary along the horizontal direction instead of the vertical direction as seen in the figure.

To produce the fringes seen in figure 30, a variety of wavelengths were used. The selected wavelengths cover the expected spectral range of our spectrometer. These are the same wavelengths used to illustrate the NSC shaded 3D model seen in figure 28. Red is 785nm, while the longer wavelengths up until 885nm are colored progressively darker.

,	W	avelengths
	۲	Settings
	۲	Wavelength 1 (0.785 um, Weight = 1.000)
	۲	Wavelength 2 (0.885 um, Weight = 1.000)
	۲	Wavelength 3 (0.830 um, Weight = 1.000)
	۲	Wavelength 4 (0.800 um, Weight = 1.000)



The main wavelength that was used in ZEMAX is the first wavelength in figure 33. Which is the 785-nanometer laser wavelength.





If you look from the zero y-coordinate along the x-direction of the detector view, note how there is an absence of a bright fringe. This is expected as the Littrow wavelength that we have set to the laser wavelength, or the first diffracted order

redirected back into the system, in which we heterodyne around does not constructively interfere. The configuration of our system appeared to function as expected. Remember, the gratings are equidistant from the beam splitter. The beam splitter is modeled with an isotropic index, meaning that the index of refraction is assumed to be measured as the same across the material. A compensator plate is usually placed to ensure the optical path lengths are the same. Considering the Michelson interferometer again, there is an additional $\lambda/2$ phase difference when light reflects from a medium of a greater index of refraction. Therefore, it is important to maintain the optical path length difference is equidistant to ensure that the two rays are in fact out of phase by 180°. Thus, the first diffracted orders from the separate gratings that are redirected back along their path incident propagation paths towards the beam splitter will destructively interfere due to their relative phase difference.

The resulting fringes seen in figure 30 are a consequence of the interaction of the variety of wavelengths used in modeling the SHS. To observe spectral information, one would take a Fourier transform of the resulting interference fringes. Should light from Raman scattering be collected into the SHS, the Raman signal would be encoded within the fringes. After an FT of the fringes, the Raman signal along with other signals within the SHS may be demonstrated on a more traditional intensity vs. wavelength spectrum.

To produce the traditional intensity vs. wavelength spectrum, one can simply take the produced image of the interference pattern from ZEMAX and perform a Fast Fourier Transform. A table of the numerical values that represent the image (as in figure 29) can be copied directly from ZEMAX.

🖉 Non-Sequential Component Editor 🥤 🖽 2: NSC 3D Layout 🥤 🚍 3: NSC Shaded Model 🥖 🗦 1: Detector Viewer X									
🛇 Settings 💈 🐚 🔛 🦯 🗌 🖍 🛏 🗛 😂 😂 3 x 4 - Standard - 🔳 🚱									
Detector Z : 80.0000									
Detector Tilt X : 90.0000									
Detecto	or Tilt Y :	0.0000							
Detecto	or Tilt Z :	0.0000							
Positio	on Units :	Millimeters							
Units	:	Watts/cm^2							
	1	2	3	4	5	6	7	8	9
1	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
3	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
5	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
6	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
7	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
8	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
9	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
10	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
12	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
13	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
14	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
16	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
17	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
<									
Graph	Graph Text Beam Info								

Figure 38 - Numerical array of the image on the detector in ZEMAX

Once this data is imported into MATLAB, the information can be converted into a type of double. First the size of the array from detector view should match the size of defined pixels as in ZEMAX. Then once this information is properly loaded in MATLAB, the image should be zero padded to provide clarity to the signal to be Fourier transformed. After this, conduct the Fourier transform upon the entire 2D array of type double and use the instruction fftshift in to bring the zero-frequency component to the center of the array. The column delimiters should be automatically set based on the file type, in our case a .txt file which contains the copied data from ZEMAX. Then the output type should be a type of Numeric Matrix. The numeric matrix is conditioned to fit the proper array size and should be square.

IMPORT	VIEW				
O Delimited	Column delimiters:	Panger 19.19	Output Type:		
• Deminiced	Tab	Kange: poso	Η Numeric Matrix 🔻		
Fixed Width	Delimiter Options DELIMITERS	Variable Names Row: 1	Text Options IMPORTED DATA		

Figure 39 - Converting ZEMAX data into a numeric matrix in MATLAB.

When importing the data into MATLAB, using the instruction imshow and dividing the overall numeric matrix by a constant such that the image is as close to the actual image in detector view via ZEMAX, the result appeared as shown in the figure below.



Figure 40 - Detector view from ZEMAX successfully integrated in MATLAB.

Note the similarity between the image of the fringes in MATLAB versus ZEMAX. Once this image is achieved, a cross section (assuming the fringes are equivalent in intensity horizontally) of the image needs to be taken and then Fourier transformed.

On the next figure, you can see an image of the cross section of the fringes that are to be Fourier transformed.



Figure 41 - Vertical cross section of fringes for image processing

The detector view is square in shape with dimension 3mm x 3mm. The fringes are not imaged perfectly to fit the entire detector, so other spatial frequencies where there are dark regions may be included in the frequency spectrum when the crosssection of the fringes are Fourier transformed. In the figure below, all the spatial frequencies are seen below centered around the zero frequency. The other peaks that are visible are the spectral components that shift with respect to that reference signal.



Figure 42 - Fourier transform of vertical cross-section with intensity vs. wavenumber.



Figure 43 - Determining the resolution of the simulated SHS.

The full-width half maximum of the designed spectrometer is seen in the figure above. As the axis is in cm^{-1} , which represents a shift in frequency from the Littrow wavelength ,the determined resolution of our system in wavenumbers is approximately $0.9919 \ cm^{-1} - (-0.5952 \ cm^{-1}) = 1.5871 \ cm^{-1}$ which is fairly close to the expected $1.67 \ cm^{-1}$ resolution from our design. This analysis via Zemax and MATLAB is done to verify the accuracy of our design.

As $1.5871cm^{-1}$ is better performing than the expected results, which can most likely be attributed to the way ZEMAX conducts its non-sequential ray tracing, one could expect the actual results of our physical spectrometer to not perform as well.

The requirement constraints that we had in place was $20cm^{-1}$ for our resolution, so with all the changes that we've placed in efforts to reduce the physical dimensions of the SHS have improved the performance overall.

<u>4.6 – Prototype Spectrometer</u>

Figures 40 and 41 of the spectrometers show the different perspectives of the prototype spectrometer. You can see the diffraction grating, a lens, and a detector.

A prototype of an ½ inch Raman spectrometer will include a compact, rugged design that can be easily integrated into the well-plate reader. The spectrometer in this case will consist of a laser source that will be connected to a fiber. In this prototype the sample will not be included in this design so far.



Figure 44: Protype of our spectrometer

The laser source provides the excitation wavelength, which will be in the nearinfrared range. The sample chamber that is in the well plate reader holds the sample to be analyzed, and the laser is focused onto the sample to excite the molecules and generate Raman scattered light.

After being collected by the lens and directed onto the diffraction grating, the Raman-scattered light is divided into its constituent wavelengths. The detector then logs the intensity of the scattered light as a function of wavelength, usually using a CCD or CMOS sensor.

High spectral resolution and sensitivity are features of the prototype 1/2-inch Raman spectrometer that enable it to identify analytes in samples with low concentrations. The spectrometer's small size makes it simple to include into handheld or portable devices for field measurements.

The prototype often uses a high-quality diffraction grating and lens. Filters or other optical components may also be added to the spectrometer to lower background noise and boost signal-to-noise ratio. Some elements will help see the true signal of the sample that we have be analyzing.

Depending on the experimental settings and objectives, it can at times be useful to reduce the signal in a Raman spectrometer.

A few situations where it would be wise to reduce the signal include the following:

To prevent sample damage, it is sometimes possible for the laser intensity used to excite the sample in a Raman spectrometer to be too high, which can result in sample degradation. The Raman signal can be lowered to a level that prevents sample damage while still giving valuable information by lowering the laser power or the detector's integration time. To prevent spectrum saturation, the Raman signal can saturate distortion or loss. The spectrometer can avoid saturation and produce more precise and trustworthy data by reducing the signal intensity. To broaden the dynamic a high signal level might also restrict the detector's range. If the detector is a valuable part of this design project. A high signal can make it harder to detect weak signals or low concentrations. The dynamic range can be expanded, and the spectrometer can detect a larger range.

All in all, it can be advantageous to reduce the signal in a Raman spectrometer in circumstances when the high signal level may result in circumstances when a high signal level may result in a spectrum saturation of the signal where we want to analyze the signals.

The prototype of a 1/2-inch Raman spectrometer also includes electronics and software for signal processing and data analysis in addition to the optical parts. This makes the Raman spectrum helpful for a variety of applications, such as material analysis, pharmaceuticals, forensics, and environmental monitoring. It also enables real-time monitoring and analysis of the Raman spectrum.



Figure 45 – Spectrometer overview

4.7 – Well-plate reader and Illumination System

The illumination system that we are using has been donated to us by our sponsor, Ocean Insight. The fibers have been by our team and catered to our system to work in the near infrared region of the electromagnetic spectrum. In a sense, our spectrometer, though designed to be more compact, can fit in the housing of the device seen in the image below.

The well plate reader can be seen in the figures below. This is the main housing of the whole project. This will keep the spectrometer and all the electrical components in one place.

The well plate reader typically includes a detector, a light source, and a mechanism for moving the microplate to read each well. The detector monitors the amount of light that goes through or is released by each well's sample, which can be used to quantify the amount of a specific chemical or to detect variations in enzyme activity.

Well plate readers are available in a variety of configurations based on the sort of measurement required. Fluorescence readers utilize a light source to excite fluorescent molecules in the sample and measure the amount of light emitted, whereas absorbance readers normally use a monochromatic light source to measure the amount of light absorbed by a sample. In our project we have a 758-nanometer laser.



Figure 46 - General overview of the illumination system.



Figure 47 - Top front view of the illumination system and general component housing

At the very top is the well-plate reader compartment, where the cuvettes are to be housed on ride a Zaber motor. As mentioned previously, the cuvettes are round but flat on the bottom. The laser light is to illuminate the sample from beneath and since the surface of the cuvette is flat, reflection or refraction off a surface of a surface of curvature is ignored.

In the drawer below the well-plate reader compartment, one can see a reflective touch screen display. Behind this is where the components will be housed. The laser, fibers and fiber connections, the spectrometer, as well as various USB connections will lie inside of this drawer. The idea is to have it all housed inside of a modular device, where the drawer is to be slid open to easily troubleshoot or access any of the components in our system.



Figure 48 - Rear view of the illumination system



Figure 49 - Overhead view of the well plate reader

Again, the laser light illuminates the sample from beneath the cuvette. The motor will be programmed to place the cuvette directly over a Raman probe. The laser light will be focused onto the sample. Since the bottom of the cuvette is flat with a negligible thickness, the refraction of the laser light is also considered in this case to be negligible.

The laser light is to be carried by a single-mode fiber, selected to be PM780-HP which has a numerical aperture of 0.12. The mode field diameter is approximately $5.3\mu m \pm 1.0\mu m$ at around 850nm. The range of wavelengths that this fiber can carry is from 770nm-1100nm.

The light emitted from fiber is then guided to a Raman probe. This probe contains a dichroic mirror and a focusing lens. We recognized the distance of the probe output coupler and the cuvette (which in this case is fixed due to the physical setup of our donated illumination system housing) to be approximately 5mm. Since the light is collimated, we can treat the 'object' as infinitely far away.

$$\frac{1}{\infty} + \frac{1}{d_i} = \frac{1}{f} \to \frac{1}{d_I} = \frac{1}{f}$$

Thus, the focal length of the Raman probe imaging lens must be approximately 5mm and operate in the NIR range.

Looking at the figure above, the way a Raman probe operates is that the light is reflected at the dichroic mirror and then focused onto the sample. This light is then passed through a notch filter. This notch filter, which has been donated to us by our Chemistry advisor, Dr. Mathieu Baudelet, passes all reflected wavelengths except for the laser/Littrow wavelength of 785nm. The remaining light may be excess stray light or other optical factors that contribute to a noisy image, as well as of course the Raman scattered light. The collection fiber is then connected to our spectrometer, where that light is processed and imaged upon

the detector to ultimately become Fourier transformed to produce the traditional intensity vs wavenumber spectrum.

A Raman probe diagram can be seen below to better visualize our approach.



Figure 50 - Raman probe schematic

This type of Raman probe is to be custom mounted underneath the well-plate reader at a fixed position. The Zaber motor will then be programmed to guide the well-plate to positions such that the fixed Raman probe position is directly beneath a specific cuvette, which is perfectly centered over the Raman probe.

As previously mentioned, the laser that we are using will be of 532 nm wavelength. There is an output for serial commands in which we can program the laser intensity, laser output toggle, as well as interlock override control. Our team was given this laser through our sponsor. The laser is connected to the excitation fiber which is then guided to the Raman probe beneath the well-plate. The collection fiber collects the scattered light from the sample and is then guided to the spectrometer. See figure 43.

The laser, laser control box, and spectrometer are all housed in the drawer as seen in figure 47.



Figure 51 - Housing compartment for system components

Of course, the drawer seen is only a prototype for visualization purposes. Cable management will be a priority. Ultimately the spectrometer will be a direct USB connection to the camera that is being used, previously mentioned. To reiterate, the USB camera being used to capture the fringes is an IDS Eye 3860CP-M. This camera is monochrome and will be connected to a USB output port on the back of the housing of the illumination system directly to a personal laptop or other computer. We would like our system to be adaptable and modular with use for several options.

Overall, the illumination system consists of the Raman probe, notch filters, and imaging lenses, as well as the collection and excitation fibers. The previously mentioned parameters have guided the spectrometer design process. As we are using a laser wavelength, or Littrow wavelength, of 532nm, this has influenced the design of the illumination system as well as our Spatial Heterodyne Spectrometer. Keeping the design of the spectrometer compact has enabled us to use the donated illumination system housing. The relationship between the spectrometer parameters and characteristic and the illumination system was a constant trade-off design wise, mostly in favor or optimizing spectrometer performance.

4.8 Sample Usage

Choosing the right samples is important in Raman spectroscopy for our project which is water analysis to be able to ensure accurate and reliable results. Water can contain a wide range of contaminants. Including organic and inorganic compounds which we would not want to see in our results because it can interfere with the analysis. This is something that we have been talking to our advisors about and how we can really understand the chemistry aspects of our senior design project.

The selection of contaminants is critical in Raman spectroscopy because different compounds have distinct Raman shifts, which are the distinctive frequencies at which they scatter light. We can identify the presence of certain contaminants in a sample by selecting specific contaminants to test based on their unique Raman spectra.

One of the great advantages of Raman spectroscopy is its ability to identify substances even in complex mixtures. Since each substance has a unique Raman spectrum, it is possible to isolate and identify individual components within a mixture, even at low concentrations. This makes Raman spectroscopy a valuable tool for a wide range of applications, from forensic analysis and drug discovery to environmental monitoring and materials science.

Some contaminants that we have shown in the optical demonstration was a substrate of sulfur and ammonium nitrate. Sulfur naturally occurs in hot springs and in other materials. The highest concentration of sulfur is found in the canal

water in the Everglades in Florida. In most cases it is relatively safe. Excess exposure can smell like rotten eggs and can cause nausea. The second contaminant was ammonium nitrate. This contaminant is commonly used in fertilizers. Excess of this can get into streams and rivers. Excess exposure can cause respiratory tract irritation, headaches, dizziness, and convulsions. Water contamination analysis is very important because it can save a life to the things that they might be at risk at.

<u>4.8.1 Sulfur</u>



Sulfur is a great contaminant to measure in water. This is because the substance has a strong Raman scattering effect. Sulfur has two distinct peaks which are at 220 inverse centimeters (798.8 nanometers) and 473 inverse centimeters (815.3 nanometers). When the sample is illuminated by the sample, the sulfur atoms in the sample will absorb the laser photons and emit a scattering effect (different wavelengths). Sulfur is a unique element that has several modes of vibrational atoms. This makes a great fit for Raman spectroscopy. Furthermore, the Raman spectra of sulfur-containing compounds are frequently unique and easily distinguishable from other compounds in the sample.

In the optical demonstration we showed the peaks of the sulfur and how easily distinguishable it is from the background noise and ethe excitation wavelength. However, with the demonstration we have did not have the sulfur in water but by the time our final demonstration is on the way we have all contaminants in water.

Sulfur is also a prevalent pollutant in a wide range of samples, such as water, soil, and industrial products. The ability to quantify sulfur correctly via Raman spectroscopy can be useful in a range of applications, including environmental

monitoring, industrial process control, and materials analysis. The concentration of sulfur in parts per million (ppm) can vary depending on the sample being analyzed. Sulfur concentrations in environmental samples such as soil or water can range from a few ppm to several hundred ppm. Sulfur concentrations in industrial samples, such as crude oil or gasoline, can reach thousands of parts per million (ppm).

To protect public health and the environment, the Environmental Protection Agency (EPA) has established safety guidelines for sulfur in water. The EPA has set a secondary maximum contaminant level (SMCL) for sulfur in drinking water at 0.05 mg/L, or 50 parts per billion (ppb). This level is designed to prevent only aesthetic difficulties, such as taste and odor issues, rather than health effects.

Furthermore, the Environmental Protection Agency (EPA) has issued recommendations for the safe handling and storage of sulfur-containing substances in water treatment plants and other facilities. Personal protective equipment, ventilation systems, and spill response plans are all required under these criteria. These requirements must be followed by facilities that handle sulfur-containing substances to protect their personnel and prevent environmental damage.

It's vital to remember that the laser power and instrument calibration can all have an impact on the accuracy of the sulfur ppm measurement using Raman spectroscopy. Overall, sulfur's strong Raman scattering effect, combined with its distinctive and complicated Raman spectra, make it a valuable material.

4.8.2 Ammonium Nitrate

Another sample that will be used in this project for analysis is ammonium nitrate. Ammonium nitrate is a suitable Raman measurable substance because of its molecular vibrational modes, which produces Raman scattering signals. One of the most prominent peaks happen at around 1050 cm^{^-1}. In the optical demonstration that was done the peak of the substrate was around 855 cm^{^-1}. A factor that could have resulted in this was the amount that was put into the cuvette. The reason for the different shifts that we see is because of the laser that was used to see the Raman shift.

This also corresponds with the compound being symmetrical in its lattice. This substrate is known the be used in various industries like agriculture and mining. Its detection and quantification are very important to ensure the safety and the regulation of safety levels. Raman spectroscopy offers a fast, non-destructive method for analyzing ammonium nitrate that will be performed in out project.



Figure 53 - Conceptual of Ammonium Nitrate Peak

The project will be heavily influenced by the right amounts of substrate we put in each cuvette. We do not want to put too much or too less of the of each substrate. In preparing for our testing of different kinds of contaminants we have a plan to test different concentrations in the cuvette. This is how we have made sure testing and calibration of the instrument is correct and has minimal error.

In our testing results unfortunately, we could not measure in parts per million (ppm) but we were able to have two different concentrations for each measurement. The figures below show the fringes and the spectrum of a larger concentration and a smaller concentration.

The Environmental Protection Agency (EPA) has not set specified the safety standard for ammonium nitrate in water. However, ammonium nitrate can be a source of contamination in water. Which can have health effects if consumed in high concentrations. The EPA has also established a maximum contaminant level (MCL) for nitrate in drinking water of 10 milligrams per liter or 10 parts per million. This level is to protect babies from a condition where their skin can turn blue because of the level of nitrates in the body. They also have guidelines for the same handling of ammonium nitrate because of the properties it has that can affect the environment and people's way of living.

In our testing results unfortunately, we could not measure in parts per million (ppm) but we were able to have two different concentrations for each measurement. The figures below show the fringes and the spectrum of a larger concentration and a smaller concentration. When using different concentrations, the larger concentration would have a higher intensity than the than the lower concentration. This is the case because since one of the vials has more concentration than the other. It has more scattered Raman signal and vibrational modes than the one with less concentration.



Larger concentration 1750mg/ml Exposure Time: 10 seconds



Exposure Time: 10 seconds

4.8.3 Potassium Perchlorate

Potassium Perchlorate is a chemical compound that is commonly used in a variety of applications. It is commonly used an oxide for different reasons. Potassium perchlorate is considered a contaminant when it occurs in the environment, particularly in water sources. The biggest issue is that it may interfere with the thyroid gland's function.

Perchlorate is chemically related to iodine, which is required for the generation of thyroid hormones. When perchlorate is consumed, it might limit iodine uptake by the thyroid gland, potentially disrupting thyroid hormone synthesis. This can be harmful to metabolism and growth, especially in pregnant women and infants.

The U.S. Environmental Protection Agency (EPA) has not set a federal Maximum Contaminant Level (MCL) for perchlorate in drinking water. They have set a proposed rule to the agency to have an MCL for perchlorate set to 18 micrograms

per liter or 90 micrograms per liter. This is a non-enforceable health advisory to protect sensitive populations like pregnant women, infants, and individuals with iodide uptake inhibition.

When a substance is subjected to a laser in Raman spectroscopy, it scatters the light, resulting in a Raman spectrum that provides information on molecular vibrations and rotational transitions. The Raman spectra of potassium perchlorate would show typical peaks related to its chemical structure. T

Raman peaks for potassium perchlorate: A peak around 1020-1050 cm-1. Which would equate to 563 nanometers to 571 nanometers. The intensity and location of these peaks would be useful in identifying and measuring potassium perchlorate in a sample. The Raman spectrum analysis provides for the quick, non-destructive, and non-contact detection of potassium perchlorate in a sample.

In our testing results we were able to have two different concentrations for each measurement. The figures below show the fringes and the spectrum of a larger concentration and a smaller concentration. When using different concentrations, the larger concentration would have a higher intensity than the than the lower concentration. This is the case because since one of the vials has more concentration than the other. It has more scattered Raman signal and vibrational modes than the one with less concentration.



Larger concentration 1750mg/ml Exposure Time: 10 seconds



4.8.4 Sodium Sulfate

Sodium Sulfate is a naturally occurring inorganic compound. It can be found in minerals. It can also be produced synthetically through various industrial processes. Sodium sulfate is not commonly regarded as a hazardous environmental contaminant. It's commonly utilized in a variety of sectors, including detergents, textiles, and papermaking. It is generally not detrimental to human health in modest amounts. However, as with any chemical, over exposure to sodium sulfate might have certain negative consequences, especially if used in high quantities. Excess salt consumption can contribute to health problems such as high blood pressure or aggravate certain health conditions.

The U.S. does not have a specific Maximum Contaminant Level (MCL) for sodium sulfate in drinking water. This is because it is considered generally a non-toxic at normal exposure levels.

Sodium sulfate is expected to produce typical Raman peaks related to its molecular structure in Raman spectroscopy. The sodium sulfate Raman spectrum will reveal information about its chemical vibrations and rotational transitions. Some typical Raman peaks for sodium sulfate include a peak near 1000-1100 cm-1 is associated with symmetric stretching vibration. This would equate to being 561 nanometers to 565 nanometers. Another peak about 400-500 cm-1, this would be 561.57 nanometers to 568.54 nanometers.

These peaks would show on the Raman spectrum if a sample containing sodium sulfate was subjected to a laser. The Raman shift represents the difference in

energy (frequency) between incident and dispersed laser light. The Raman spectrum analysis can be used to identify and quantify sodium sulfate in a material.

It is important for us to follow these guidelines when thinking about our project design and how it would relate to the real world. We must abide by our standards and specifications when doing the contaminant picking. One of our advisors is a chemistry professor. So, he was able to guide us and give us assistance on which would be beneficial for this project.

Other contaminants that will be considered in measuring would be chloride, oil, and hydrocarbons. Chloride is a common contaminant in both freshwater and seawater. This contaminant can have harmful effects on an aquatic ecosystem. Raman can accurately detect chloride levels in water, allowing for effective monitoring in the water.

Also, oil and hydrocarbon contaminants have significant impact on aquatic ecosystems and the human's health. Raman spectroscopy in this case can also be used to monitor the water.

Finally, Raman spectroscopy is an extremely effective analytical tool for detecting and characterizing pollutants in water samples. The selection of appropriate contaminants is critical for the analysis's accuracy and sensitivity. Compounds with strong Raman signals, such as ammonium nitrate and sulfur, can be easily detected in water samples using Raman spectroscopy.

Cuvettes, fiber collimation, and a suitable imaging system are also required for reliable and reproducible results. Overall, Raman spectroscopy is a quick and non-destructive technology for water analysis that has the potential to be widely used in a variety of sectors and academic fields.

In our testing results unfortunately, we could not measure in parts per million (ppm), but we were able to have two different concentrations for each measurement. The figures below show the fringes and the spectrum of a larger concentration and a smaller concentration.

When using different concentrations, the larger concentration would have a higher intensity than the than the lower concentration. This is the case because since one of the vials has more concentration than the other. It has more scattered Raman signal and vibrational modes than the one with less concentration.





Smaller Concentration 550mg/4ml Exposure Time: 10 seconds

4.8.5 Conclusion

The Raman shift is the difference in frequency between the incident laser light and the scattered light, and it is affected by the vibrational modes of the sample molecules. Each chemical bond in a molecule has a distinct vibrational mode, which results in a distinct Raman shift. As a result, evaluating a sample's Raman spectrum can reveal useful information on the sample's chemical makeup.

To minimize this interference with the results, it is important to carefully select samples that are representative of the type of contamination being analyzed. Another thing that we talked about in the constraints and standards part of this paper is that is it also important to prepare and handle the samples.

It is crucial, however, that Raman spectroscopy cannot identify all pollutants. Some compounds might not display notable Raman scattering or may exhibit faint signals
that are difficult to detect. Furthermore, the sensitivity of Raman spectroscopy can differ depending on the instrumentation and sample preparation methods used.

As a result, the pollutants we choose should be chosen for investigation based on their ability to be identified by Raman spectroscopy and their relevance to the specific application. To achieve precise and trustworthy results, proper sample preparation techniques and equipment calibration should be used. Since we have a chemistry advisor, we can ask for guidance and assistance with which contaminants are good or not for Raman spectroscopy.

During the process of senior design two (SD2) many of these methods will be turned into conceptual to hands on. Many of the optical and electrical components that we have talked about in this project will be shown and turned into an actual product in the months to come.

4.8.1 Testing and Validation

To test our spectrometer, we attempted to retrieve the spectrum of Mercury. By simply inserting a Mercury light source via FC/PC fiber into the spectrometer, we obtained the below interference fringes. When Fourier transformed, the spectrum of Mercury is also obtained.



Figure 54 – Mercury fringes from our SHS Fourier Transformed to produce the Mercury Spectrum.

We were able to observe the spectrum of Mercury and were able to compare to NIST standards to determine if our results were accurate, however the wavelength axis is not properly configured to determine the true intensity versus wavelength relationship.

Calibration of a Raman spectroscopy system is critical and is an essential process that ensures the accuracy, reliability and repeatability of the measurements taken by the spectrometer.

Calibration creates a direct link between the measured Raman shifts and the reference materials' real vibrational frequencies. This precision is critical for precisely recognizing and quantifying the chemical components present in a sample. Without proper calibration, the Raman shift results may contain mistakes or inaccuracies, leading to inaccurate interpretations of the sample's composition. Raman spectroscopy is used for quantitative analysis in some applications, determining the quantities or amounts of specific substances in a sample. Calibration is required to transform measured intensities into consistent concentration values. The quantitative results may be untrustworthy if the calibration is not precise.

Overall, calibrating a Raman system is a critical step in generating consistent and relevant findings from the technology. It enables a wide range of applications, from fundamental research to industrial analysis, ensuring data precision and repeatability and allowing Raman spectroscopy's full potential to be fulfilled in diverse scientific and technological domains.

To test, we had to calibrate using a known light source whose range is within the range of our spectrometer, which is expected to be about 100nm. This light source also needs to be a line source to better assess what wavelengths we have present on the detector. The light sources we had selected which was Mercury.

To test, calibrate and validate, the light source is inserted, the fringes are to be inspected (SHS may need to be continued to be fined tuned in alignment), save an image, Fourier Transform the image from row to row and average, and plot the peaks against the number of pixels on the detector. A good statistical minimum is picking three peaks that are strong and distinct. It's preferred to pick peaks that are singlets, as opposed to doublets.

Once the pixel position of the peak is determined, where the x-axis is the pixel position and the y-axis is the peak position in nanometers, one can acquire a linear calibration curve in the form of y = mx + b. Once this equation is obtained, one can enter a pixel number into x and retrieve a y value. Below is an image of Mercury's peak vs pixel plot as well as its linear calibration curve. The know peaks of Mercury is 546nm, 576 nm and 579 nm.



Figure 55 - Intensity versus detector pixel plot as well as calibration line for Mercury

By following this procedure, one can obtain a calibrated x-axis for all wavelength within the spectral range. The measured resolving power for our SHS using Mercury was 6000, while the actual spectral range is 86.284nm, which is equivalent to 2620.58 cm^{-1} . Peaks that shift by $800cm^{-1}$ and lower are weak and our SHS may not be sensitive enough to pick them up. Our resolution is 0.4683 nm. Calibration is also not perfectly set.

Moving forward to our chemical analysis, we first tested with Sulfur. The resulting fringes and plot are seen below.



Figure 56 - Sulfur fringes on the left (see closely to observe fringes) and resulting spectrum on the right. 797.3nm peak is extremely close to the anticipated Sulfur Raman peak, while 801.7 is off from the expected 810nm Raman peak.

While the 797nm peak is extremely close the expected 798nm Raman peak, the 801.7nm peak is in the wrong location. By comparing to other Raman measurements, we know that this peak should be at approximately 810nm. See figure below.



Figure 57 - Raman spectrum of Sulfur. Image from <u>https://www.researchgate.net/figure/Raman-spectra-of-</u> <u>raw-technical-sulfur-and-reference-sulfur-sample_fig6_284479743</u>.

The peaks of interest of $220cm^{-1}$ and the $246cm^{-1}$, which correspond to 798nm and 810nm on a wavelength scale respectively.

5.0 Constraints & Standards

This section will follow details about constraints and standards applicable to our system. The standards section describes the guideline which the product will be engineered. The constraints section describes which the SHS must follow. By complying with these standards, will make sure that the product will be built safely so the consumer can use it and is not dangerous.

There will also be information on the standards to follow for our electrical components. This includes standards for any PCBs that we design, the batteries that use to power the various components that require their own power supply, MATLAB coding standards, power consumption standards, and any general standards that must be followed when designing electrical machinery.

These will generally be outlined by IEEE, and we have closely followed such standards to ensure that our design is fully capable to be used on the open market. Our goal is to design something that is capable of being sold or used by any company that would need the services provided by our system.

5.1 Design Standards

A standard is an established way of doing things that ensures the instructiveness between the components. Without engineering standards, the use of technology in the engineering industry, including the SHS would be limited and hard to follow. The vast differences in how goods are designed, and run would result in severe market mismatches. If there were no standards, products that ought to go together naturally.

Standards guarantee the health and safety of those who use and handle the product daily. Moreover, standards guarantee that the product is secure and will not hurt users. Professional engineers and organizations that certify standards say that adhering to and defining standards helps with engineering practice.

5.1.1 Power Supply Standards

The system that we are using requires multiple power supplies to power various components throughout the system that is vital to the overall success of our project. Some of these components include the laser, the motor that controls which cuvette is having the laser shot through, the spectrometer, and the computer that controls all those things and gathers the data. With that said, having multiple power supplies the standards for power supplies must be observed. The main standard is the IEEE 2847-2021 standard that covers "IEEE Standard for DC Power Transmission and Communication to DC Loads" (IEEE, 2022). The standard describes how to properly implement the distribution from a DC power source to multiple other DC loads. It describes how the DC power should sent from the transmitter to the loads along "a pair of power lines in in a multidrop bus or tree topology".

Part of the reason that these standards were developed was so that engineers attempting to power something would know the proper practices to adding a power supply to a system. One of the topics that are highlighted in the standards are about the distribution of voltage from the DC power supply to the components that require power to function. By developing and standardizing a safe method for distributing the current. The standard states that the DC power supply (that is receiving a high level of voltage from the grid) is correctly reduced and distributed to the other components of the system. If this is not done properly, the components risk overheating and being damaged past repair. Furthermore, this could cause bodily damage to those around the part as it overheats in case it violently explodes. One of the components that we must pay special attention when giving it power is the laser. If the laser were to malfunction there could be serious problems and the supplying the laser with the right amount of power is the first step towards ensuring the safety of our team and any users in the future. Another reason that abiding by the guidelines laid out for us in the standards is of crucial importance is that getting the right cables for the voltages flowing through them is essential to a fully functional system. While there is another safety aspect involved in terms of things overheating and melting, getting the right cables allows for us to ensure that there is not too *little* power flowing to our components. This is for obvious reasons but if the voltage is not high enough to turn on the part, then our spectrometer would not only simply not work but there is another possibility for bodily harm if there is enough voltage for a machine to run but not enough for the cooling fan to start. Cooling fans will be vital in our system because the entire thing will be enclosed in a metal compartment and the laser itself generates enough heat for smaller wires and miscellaneous components like resistors to fail.

Following the standards outlined in IEEE 2847-2021 allows us to safely and efficiently allocate enough power to all our components without using up too much power or overloading our components that could in turn cause more problems for both our components but also the source for our DC power supplies. Not to mention that if we want to sell this product, we have need to be compliant with all relevant standards to receive a sort of "seal of approval" from IEEE that will open the market up to more buyers.

5.1.2 IEEE 802.3 Standards

To receive the data over to the computer we have be using a wired connection to transmit the data from the spectrometer. This connection can also be part of a local area network or LAN. A LAN is a collection of devices that are connected to each other within a short area; usually limited to just one building such as a home or an office. The connection types can be either wired or wireless and comprised of cables, computers, routers, ethernet switches, and anything else that is capable of being connected from one device to another (Cisco, n.d.). The Institute of Electrical and Electronics Engineers Standards Association developed a set of standards for the use of local area networks that gives guidelines on how to properly set up one of these networks and make it as efficient and easy as possible to connect to the network (IEEE, 2018). It also defines the physical and MAC addresses of the data link layer for the wired Ethernet networks. The reason we are using the wired standard is because that is the easiest way for us to connect all the components of our system. Wired connections are also often easier to connect, easier to troubleshoot, and more reliable than a wireless connection. There are also sections of the standards that describe what kind of capabilities the devices that are connected to it must have to fit into the standards and thus be able to be part of the network.

These specifications are more things that we must take into consideration when we are deciding what parts to choose when we are building our system and the supporting components. Some of these specifications affect the way that the information is transmitted as well as how quickly they are transmitted. For example, the standards describe the relationship between the size of the frame and the length of the cable that connects the two. Information is sent over as a series of bits that are called a frame. The minimum size of a frame is 512 bits or 64 bytes and as a result the maximum length of an ethernet cable is 500 meters. The reason for this is that if the cable is any longer than that there is a possibility that the signals that you send over can be crippled by the existence of too many, uncaught collisions (Propagation Delay and Its Relationship to Maximum Cable Length, 2019). Collisions are when the two machines that are connected by an ethernet cable send information across the cable at the same time. If the cable is less than or equal to 500 meters in length; either one of the stations will notice that the collision occurred, and it will naturally correct the problem. However, if the cable is too long, there is an increased chance that the collision will go unnoticed, thus resulting in garbled signals that are from what the user expected to receive. This is one of many specifications that are set in the IEEE 802.3 that we must adhere to when designing our system because otherwise our system could crumble from simple data miscommunications.

5.1.3 IPC PCB Standards

Our spectrometer will include a few key PCBs to complete various objectives that we have laid out for ourselves. One of these goals is to create a safety interlock that would prevent the door with the laser from being opening when the laser is one and if the door does become open the laser immediately turns off. More on this mechanism in a section down below but because we are making a PCB, we must adhere by the standards designed for us by the Association Connecting Electronics Industries. The reason that these standards are useful to us is not necessarily because they guarantee our safety (those safety measures are outlined in other standards) but rather to ensure that we design quality PCBs. IPC creates standards but is a non-profit organization with members that span every part of electronics industry which allows them to create standards that are used throughout and ensure that professionals utilize these standards despite not being as official as say IEEE.

IPC's standards outline things like how to choose materials that will maintain the electrical, mechanical, and structural integrity of your design. They also outline what the board itself should be built with and how to choose what kind of adhesives and plating to use. The standards are also great for figuring out the dimensions of your board and how they could affect the performance of it. And some characteristics of the board that most people often overlook are also considered in their standards. Their standards also extend to the software that is used to design PCBs like Altium, and Eagle. This what makes the computer give us warnings when designing a PCB that the action we are attempting to make will hinder the performance of the board. By being a member-driven organization the standards that are set are not only developed by their members, but their members also bring in the companies that they work for. By doing so, these companies adopt the standards and make them a guideline for all their employees, which further pushes

the standards set by the IPC to be used throughout the industry (Generic Standard on Printed Board Design, 2003)

Following the standards of IPC for PCB design is crucial to any engineer attempting to create something that will be bought and used throughout the world. We want to design and build something that is reliable, quality, and performs its intended purpose to perfection.

(Generic Standard on Printed Board Design, 2003)

5.1.4 RoHS Compliance

RoHs stands for Restriction of Hazardous Substances and impacts the entire electronics industry and many products as well. This standard is primarily found in the European Union electronics to protect the environment and public health. Protecting people's health and the environment from potentially dangerous chemicals produced during the manufacture, use, and disposal of electronic equipment is the goal of RoHS compliance.

A wide variety of EEE products, including home appliances, Computer equipment, lighting products, medical devices, and monitoring and control instruments, must comply with RoHS regulations. Manufacturers of EEE must make sure that their goods don't contain prohibited compounds over the maximum concentration values to achieve RoHS compliance. This entails testing and certifying finished products in addition to the careful selection of suppliers and materials. Significant fines and other legal repercussions may follow from failure to comply with RoHS requirements.

This RoHS standard has been evolving into a global standard for many businesses that use electronics. This is a way to help not only the environment but have sustainable production methods.

5.1.5 Laser Safety Standards

The use of eye protection is advantageous for almost every sector, especially when you are dealing with lasers. When using lasers, eye safety is of utmost concern because laser radiation exposure can hard the eyes permanently. The lens can concentrate the laser beam onto a small region on the retina which can result in a thermal or photochemical damage to the human eye.

The severity of the eye injury can depend on several factors, including the wavelength of the laser radiation, the power density, and the size of them beam spot. Lasers are classified for safety purposes on their potential for causing injury to humans. As a result, the following is a working list of the SHS standards that have mist be considered into considerations. Each standard will be explained of

how it relates to the project. A review of the postulated and actual engineering limits for the SHS follows the section on standards.

5.1.5.1 Class 1 Lasers

• These lasers are safe for the eyes because they usually have a very low output power. Which is only a few microwatts.

5.1.5.2 Class 1M Laser

 Class 1M lasers are like class 1 but the difference is the that they cannot be viewed from a magnified source. By doing this the laser can be amplified. This type of laser you can look at the bean without eye safety without being harmed.

5.1.5.3 Class 2 and 2M Lasers

- This class of lasers is dangerous because the light is visible.
- Like class 1M class 2M cannot be viewed from a magnified object. This can cause severe eye injuries when viewed for too long.

5.1.5.4 Class 3R and 3B Lasers

- Class 3R lasers are types of products like laser pointer and laser scanners because they pose a higher safety risk than the other classes.
- With laser class 3B lasers direct contact with the lasers themselves or specular reflections must be avoided at all cause. This can cause eye injuries and small burns.

5.1.5.5 Class 4 Lasers

• This class is the most dangerous because the output power is so high that it can ignite materials and can cause more damage to the eye and skin.

From all the laser hazards, the most serious are eye injuries. The main reason this is the case is because the eye lens acts as a natural amplifier. With skin hazard, it's not as bad as hurting your eyes but it can cause burns.

As scientists realized that even low-power lasers could be potentially harmful, laser standards were first established. To avoid health and fire risks, they offer the proper laser safety precautions. The many classes, how to compute certain laser parameters, appropriate labels, safety precautions when handling the laser, and other topics are all covered in all which specifies the hazardous areas of direct laser light, specular reflections, and diffuse reflections.

To prevent eye injuries from lasers, it is important to use appropriate eye protection, which can include goggles or glasses that are specifically designed to

absorb or reflect the laser radiation. The eye protection should be selected in accordance with the precise laser's wavelength and power, and it should conform to the required safety regulations, such as those set forth by the American National Standards Institute (ANSI) or the International Electrotechnical Commission (IEC).

The **international standard** is **IEC 60825-1**. The International Electrotechnical Commission (IEC) created the technical standard IEC 60825-1, which outlines the safety criteria for laser goods, including laser systems used in industrial, medical, and consumer applications. The standard specifies standards for labeling and user instructions as well as guidelines for evaluating laser dangers and categorizing lasers according to potential hazards. For lasers to be used safely and to avoid harming people or the environment, IEC 60825-1 compliance is essential.

The North American standard is **ANSI Z136** offers recommendations for the secure application of lasers. It was created by the American National Standards Institute (ANSI) and covers a variety of laser safety-related topics, such as hazard assessment, protective gear, and training standards for laser operators. Regulatory agencies, and other parties involved in the laser business needs to have their standards go through the compliance of ANSI Z136. The standard is created to assist firms in establishing efficient safety for laser systems. Furthermore, these standards also require safety systems to be implemented in our design, which we have do given that our sponsor would like to use our design as a prototype that they could bring to market in one form or another.

In the USA, the FDA shows that the laser **Code of Federal Regulations Title 21**. Title 21 of the Code of Federal Regulations, which is issued and implemented by the Food and Drug Administration, governs laser regulations in the United States (FDA). The FDA regulates a variety of products that employ lasers, including consumer goods like laser pointers and light show projectors as well as medical equipment that use lasers for diagnostic and therapeutic purposes. To ensure that lasers are used safely and effectively, the rule specifies requirements for laser safety performance standards, labeling, and user instructions. FDA enforcement actions, such as product recalls, fines, and legal action, may be taken in response to non-compliance with its regulations.

5.1.6 Electrical Safety Standards

There are several electrical safety standards involved in any electrical engineering development. These range from ensuring that electrical equipment is correctly installed and does not have faulty components already in it, to wearing the right protective gear when around dangerously high voltage levels.

An extremely common and one of the most lethal electrical hazards in the workplace is the arcing. Arcing is when electrical current flows through the air from one point to the other. This can be extremely dangerous since the heat and current

can burn and even kill anyone that meets it because so much voltage is concentrated in a small area. Arcing isn't only a danger to the people directly around it, but it can also cause electrical fires to occur where they originated. Arcing most commonly occurs when a circuit is overloaded (Arcing, 2021). Similar electrical dangers are when water or some kind of conductive liquid is near an electrical circuit. The current can travel along the liquid and potentially electrocute someone. The IEEE standard IEEE 1584-2018 "IEEE Guide for Performing Arc-Flash Hazard Calculations" is a fantastic guide to ensuring that anyone working with electricity will not risk being injured by an arc-flash.

When designing our system our top priority will be to ensure the safety of the user. The last thing we want is for our users to use the machine and end up getting hurt or worse. For that reason, we have made certain that all connections are secure and will not shake loose. This prevents any possible current leakage into the metal enclosure and preserves the safety of, not only the other components in our system, but also the safety of our user. Ensuring that the connections are secure gives us peace of mind that no one will be electrocuted when using our machine. We also must make sure that our cables are rated for current that we have be pushing through them. Again, when current is too high certain components of the system (like the cables) can melt and destroy the integrity of our spectrometer. Additionally, the damaged cables could also electrocute our user or burn them if they become too hot.

Something else that we must keep in mind when working with this system is that all components are securely fastened to the enclosure to prevent the components from sliding around. If the components move around, they could become damage or damage other components that could, in turn, create unknown electrical hazards within the sealed enclosure. Also, if the components become damaged and start leaking electricity to the system, other parts of the system can be come damaged without the user knowing it and essentially render the spectrometer useless from irreparable damage.

These safety measures are not just for the user but also the team developing it. While trouble shooting, we must ensure that all connections are secure, we are not touching live wires and are well-aware of our surroundings.

<u>5.1.7 ISO 9001</u>

The ISO 9001 certification is an internationally recognized standard for Quality Management Systems (QMS). It is an issued standard by the International Organization for Standardization (ISO) and sets the criteria for management systems that ensures consistent product quality, customer satisfaction, and continuous improvement of technologies. This standard is applicable to organizations that we have be dealing with such as PCB vendors and it is a

standard that we have be seeking in our vendor manufacturer selection, this also includes companies responsible for the manufacturing of individual electrical components that will go in our design project.

The ISO 9001 is an indispensable standard to look for as it determines consistent quality. By following the ISO 9001 standard, a PCB vendor demonstrates their commitment to maintaining a high and consistent level of quality in their manufactured products. This is crucial for electrical engineering projects like ours, as it ensures that the PCBs and components, we spend money on a therefore receive perform as expected and meet the required specifications as needed.

The certification requires organizations to identify, act on and manage risks associated with the processes that go behind the manufacture of products as well as the product itself when finalized. This proactive approach to risk management minimizes the potential issues with and ensures that PCBs used in our project are less likely to suffer from defects or failures as we have not been at a great standpoint to fix big board issues, nor turning over boards that may take time that could be used in the troubleshooting and testing of the system.

Organizations holding this certification must continually evaluate and improve their processes, products, and services to maintain their certification. Therefore, the fact of seeing this certification in a vendor can give us peace of mind that we are dealing with active and evolving technologies to be used on our design. The focus on continuous improvement ensures that the vendor will stay up to date with industry best practices, leading to better PCB quality and performance over time. Companies are also required to check on their own suppliers as their material is more often also purchased from other vendors for manufacturing of PCB which can help ensure that the materials and components used in your PCBs are of high quality and sourced responsibly. This will contribute to the ultimate reliability of the printed circuit board and the functionality.

In conclusion, by browsing for ISO 9001 certified companies we are confirming the consistent quality, risk management, satisfaction as costumers, continuous improvement, and timing that our design may take to be designed. This will be the most important factor in PCB vendor selection. (Standardization)

5.2 Design Constraints

Constraints on design are limits or limitations placed on the design process by both internal and external sources. Every employee in the company must be aware of these restrictions and keep them in mind before beginning any project since they have an influence on the outcome. Another constraint is that the project is sponsored.

5.2.1 Economic and Time Constraints

5.2.1.1 Economic

Economic constraints are a good aspect to talk about regarding or senior design project. We have been sponsored by Ocean Insight so some of the financial burden has been taken off. Some of the optical components that was going to be bought would have cost a few hundred of dollars. However, great care and deliberation must be taken to pick the best electrical and optical parts that would be best for our project. The optical parts will be discussed with the engineering team. The parts that most likely will be chosen will be more expensive because it will be most likely funded from the company.

Many of the electrical and optical components can come run into the thousands of dollars. Even though the project is sponsored we still have a rough budget of the amount that the group would like to spend. The budget for our device will be roughly limited to approximately ~\$2,500, will includes all components, electronics, hardware, software, optics, and materials that would be used. Many of the optical components are expensive because of the manufacturing components and the specification that are used to make an optical system work. Since this is an approximation, we are not sure if the budget will be met or exceeded.

5.2.1.2 Time constraints

Time constraints will be one of the biggest and challenges for our team to overcome. The time allotted is two semesters to research, design, build, test and iterate and present our device. Since our group is in the fall to summer graduation time. Our time to get everything done is decreased by some weeks. During this time, since we all have other obligations in our schedules. We must commit time every week to we can progress in the development of our project. A danger that is close but far is procrastination or having bad time management, by have these two ideas it can be very difficult to get anything done. If this is done throughout the whole semester, then then we could get a failing grade for our project.

The possibilities for our design can be endless because we could design the spectrometer and the PCB in so many different types of ways. The spectrometer could analyze multiple different things, so it was good that we have a scope limited to what we want to do. This way we cannot have unrealistic features or expectations imposed on our project. Time constraints related to milestones and deadlines for this project are dictated by the senior design curriculum. By the end of the first semester, we should have our design competed and a prototype built.

At the end of senior design two, everything that is included in our project would need to be completed; design done and ready to build. Having a printed circuit board will need to be done and ordered as soon as possible because it will require a couple of weeks from the time the board is ordered to arrive. The PCB will most likely need to be ordered again because it may have errors and need to be ordered and designed again.

5.2.2 Environmental, Social, and Political Constraints

5.2.2.1 Environmental

Environmental constraints are factors in which the testing and development of a device limited by its surrounding environment. The contaminants that we are discussing to use is transition metals and bacteria. There must also be little to no natural or randomly polarized light interfering with the samples. This is because another aspect of our project is to use some natural fluorescence for the bacteria.

However, our device will be used to test and monitor water analysis so it should be able to be used for any sample in an environment where water extraction is possible.

Another environmental constraint to consider is how the samples will be obtained. We need to be careful that the contaminants, especially bacteria, does not spread. The cuvette that will store these water contaminants will be closely monitored and stored in a safe place when not used. We are only testing samples that can be used be found in the environment that close to us.

5.2.2.2 Social

Social constraints are patterns of societal and cultural behavior which can impede the development of the devise. The SHS does not have many major social constraints limiting it. It just needs to abide by standards that have talked about previously in this paper so no one will get hurt and our project does not have to suffer.

5.2.2.3 Political

Political constraints include the limitations on the project placed by the government policies and political weather in the are the project is being designed in. The terms for this project were to help with water analysis in different areas that water is located. When doing research about this topic I concluded that there are no political constraints around this topic.

5.2.3 Ethical, Health and Safety Constraints

It is vital that we carefully consider the ethical, health, and safety constraints associated with our design. These considerations not only protect the well-being of users and the environment, but also ensure that our project adheres to industry standards and regulations. The use of many optical devices such as lasers bring on the most responsibility to be had when handling the devices as users as well as designing the project keeping in mind usability and safety for manufacturing and later usage.

As upcoming engineers, we must act responsibly and consider the potential consequences of our work. Ethical constraints are poplar bashed for engineers. So many guidelines must be considered such as respecting intellectual property rights, considering the privacy and security of end-users, and ensuring that our solutions fit all possible users. By adhering to ethical guidelines, we demonstrate our commitment to creating technology that benefits society, without causing harm or perpetuating injustices and an overall successful project.

Health and safety constraints are of highly importance when working with potentially hazardous components, such as lasers and other optical devices that are at use within our design. We must adhere to international safety standards and guidelines, such as the industry standards set by the corporations in charge of looking out for the guidelines to follow that are described within this paper. These guidelines ensure that our designs incorporate features to protect users from accidental injury, such as the latching device for the laser.

5.2.3.1 Ethical

The practice of wastewater surveillance is decades old, going back as far as the cholera outbreak in 1854 and more recently used during the COVID-19 pandemic. Testing wastewater can be used to keep track of and narrow down where a disease is spreading from and how badly the disease is spreading. Similarly, an unnatural water contaminant polluting a water source can be tracked down to its source to hold those at fault accountable for their actions, close off the contamination source, and determine how much the contaminant has spread. Our project could be used for such objectives but there are some ethical considerations to consider as well.

While there may not seem like there are many ethical issues to a system that checks for water quality; there are still some constraints that we must keep adhere to when designing our system. The most notable ethical constraint is to make sure that the water samples we are testing are taken from sources that will not cause issues in the community. Not all people want their water tested since it may reveal some sensitive information about their habits that they may not want shared. Additionally, if the water sample appears to be contaminated with something dangerous; there could be serious repercussions that the community would not

want to deal with. For example, cutting off their water supply and requiring them to use bottled water for drinking and going to other places to bathe or cook food. These are ethical problems because not all people have the means to buy an indeterminate about of bottled water or be able to move to a different location for basic human needs.

Another ethical constraint is our responsibility to be honest when we are testing water. Whether it be for research or more paramount situations like court cases, we must be honest with the results as it could lead to serious consequences. That being the case, water samples cannot be artificially contaminated by the user and samples must be handled with the utmost precaution lest we cause unnecessary repercussions. This is of utmost importance because if a sample is contaminated after it was taken, there could be the issue of creating a false positive result that may cause panic over what the result entails.

It is important to make sure the spectrometer is risk-free to operate and doesn't endanger anyone or the environment. This entails making certain that the materials employed are non-toxic and that the gadget is constructed in a way that lowers the likelihood of mishaps. If we were able to take water samples from a private property to evaluate using a spectrometer, we should get permission from the property owner. Moreover, make sure that any private data gathered for the analysis is kept private.

The spectrometer's potential effects on the environment should be considered. This involves making sure the tool has no harmful environmental effects or contributes to pollution. Finally, we should make sure that the spectrometer is used morally and that it does not support any unethical behaviors like water theft or illegal dumping.

Finally, there is the ethical consideration that our water quality spectrometer system does not violate or infringe on any existing patents. If we were to violate any of these patent protections then the owner of the patents could potentially stop us from making, selling, or using our system with approval to do so from the owner. We plan on taking this very seriously and will tackle this issue by ensuring that every system we create does not have an existing patent on it. Our goal is to create a product that can be sold and used throughout the world, so we have work diligently to make sure that patent protections do not inhibit our success.

5.2.3.2 Health and Safety

The health and safety of getting the contaminants is a key and pivotal point in our design. Different contaminants have different percentages of toxins that are harmful to the environment and humans. Lead pipes, faucets, and plumbing fixtures are the main sources of lead in drinking water. Lead may be present in some water pipes that transport drinking water from the water source to the house. Lead may also be present in household plumbing fixtures, welding solder, and pipe fittings manufactured before 1986. The United Stated Environmental Protection Agency (EPA) sets legal limits on over 90 contaminants in drinking water. The legal limit for a contaminant reflects the level that protect human health and the water systems can achieve using the best technology, which in this case would be our water analysis spectrometer.

There are several Environmental Protection Agency regulations relevant to drinkable and non-drinkable water. There is the Clean Water Act, which regulates the discharge of pollutants into surface water, groundwater, streams, and wetlands. The Oil Pollution Act regulates oil spills, including those that occur in non-drinking water sources such as oceans, rivers, and lakes. The Safe Drinking Water Act primarily regulates drinking water. It also sets standards for certain contaminants in non-drinking water sources, such as groundwater.

National Primary Drinking Water Regulations are legally enforced on public drinking water systems to protect public health. For example, community water systems that contain fluoride can exceed the secondary standard of 2 mg/L but cannot exceed 4.0 mg (about half the weight of a grain of table salt)/L and must provide public notice within 12 months of learning about the exceedance (Agency, 2023).

Below is a table describing maximum contaminant level goal (MCLGs) and effects of some common contaminants by consumption ranging from organic and inorganic chemicals to disinfectants taking directly from the EPA.

Contaminant	MCLG (mg/L)	Effect	
Chlorite (disinfectant byproduct)	0.8	Anemia, nervous system effects	
Chlorine (disinfectant)	4	Eye/nose irritation	
Arsenic (inorganic)0Skin dar00circulatorycancer		Skin damage, circulatory issues, cancer risk	

Fluoride (inorganic)	4	Bone disease, mottled teeth
Nitrate (inorganic runoff from fertilizer)	10	Infant illness, shortness of breath
Ethanol (volatile organic)	0	Water soluble and negative impact on environment as well as a variety of health effects

Table 15 - Common contaminants, safe levels, and effects if overexposed.

The purpose of this subsection is not necessarily to explore the variety of contaminants in drinkable and non-drinkable water, but to emphasize the seriousness of the issue of protecting it. There are a vast number of contaminants that can be present in our water, and consequently there are a variety of technologies and techniques suited to handle its detection and treatment.

Some contaminants cannot be tasted, seen, or smelled in drinking water. The best way to know the risk is to identify the source of the water that can potentially be contaminated. Another contaminant that is not seen mostly seen in water is bacteria.

5.2.4 Manufacturability and Sustainability Constraints

These are two essential factors that we must consider in our senior design project. These factors are crucial not only for the success of our projects, but also for their long-term impact on society and the environment as we believe it to be the goal of Ocean Insight as well as our sponsor when giving this project to us.

Manufacturability refers to the ease with which a product can be produced at a large scale. As we design our projects, we should consider how the components can be easily manufactured, assembled, and maintained. By focusing on manufacturability, we ensure that our designs are cost-effective, reliable, and accessible to a greater scale by keeping in mind the global electronic component shortage. This, in turn, enhances the project's chances of adoption in the market and its potential to make a meaningful impact.

Sustainability, on the other hand, emphasizes the environmental and social impact of our designs. As future upcoming engineers, we have a responsibility to develop solutions that not only meet the needs of today but also consider the future. This includes minimizing energy consumption, using eco-friendly materials, and ensuring that our projects can be easily recycled or disposed of without causing harm to the environment, many guidelines are imposed that we go through in this paper that are set to follow these factors. Incorporating sustainability in our design projects also allows us to consider the ethical implications of our work.

5.2.4.1 Manufacturability

Manufacturability is an important aspect to consider when designing a senior project for a water analysis spectrometer. One of the things to consider is that the materials that will be used for the spectrometer like the casing, lenses, and other components. Some of the materials that will be used can be readily used and affordable if this is a project that wants to be seriously done. The material can be sourced from a supplier with some time to find everything that is needed. The manufacturability of this spectrometer is highly likely for the company that is sponsoring this project. Ocean Insight wishes to use this spectrometer prototype to be able to help with future endeavors to be able to use this a water analysis spectrometer.

The assembly needs to be considered for the ease of assembly for the spectrometer. The components will be easy to put together once we have all the lenses and the parts to be able to put it on an optical system. The components won't need to be assembles by a specialized tool or an equipment. The assembly will not be automated to increase efficiency but will have to be built by hand. The testing of the spectrometer needs to be considered for accuracy and reliability. Since, the sponsor of this project is Ocean Insight. They have a variety of ways that the project can be tested to make sure that the spectrometer works and it able to do its job effectively.

The scalability of the design can be scaled up to accommodate larger production runs if it were to come down to that from the company. The cost will also need to be considered when manufacturing the spectrometer on a larger scale. At this point right now, there is not a way to show if there are any potential cost-saving measures that can be implemented when the cost of the many spectrometers in the market are very expensive for what they do.

5.2.4.2 Sustainability

The sustainability of our senior design project depends on the factors such as material used, the energy consumption during the operation if it wanted to be scaled to a production. Also, the maintenance requirements, and the potential for recycling or repurposing at the end of its cycle as a project. Designing with sustainability in mind can help minimize negative environmental impacts and increase the long-term viability if the project.

A sustainable spectrometer should be made with high-quality, long-lasting components that need less upkeep and repair from a design standpoint. Additionally, it should be energy-efficient, utilizing less power while in use and

including energy-saving features like automated shut-off. A sustainable spectrometer should be made from environmentally friendly, non-toxic, easily recyclable components that do not harm the environment. This entails avoiding the use of dangerous chemicals and reducing production-related waste.

The operational efficiency of a project spectrometer, which includes elements like accuracy, precision, and speed, is another aspect that affects sustainability. A high-quality spectrometer that delivers rapid, accurate measurements will last longer than one that necessitates frequent calibration or yields unreliable findings. Finally, it is crucial to think about a project spectrometer's end-of-life disposal to assure its sustainability. To have as little of an environmental impact as possible, the spectrometer should be made so that it is simple to disassemble, recycle, and reuse its parts. A sustainable project spectrometer is one that is long-lasting, made of environmentally friendly materials, energy-efficient, promptly delivers accurate and exact measurements, and is simple to recycle after its useful life.

5.3 PCB Vendors / Manufacturers

Browsing for the perfect PCB vendor for our project is critical part for the success of the overall project. It may directly affect product quality, reliability, and costefficiency as well as timing since for we are dealing with limited time in the class. A perfect vendor & manufacturer will ensure that our PCB is manufactured to the given specifications and delivered on time, which in turn can help peace of mind, improve the overall potential of the board as we have had more time to troubleshoot and test for any problems that may arise.

Keeping in mind qualities that are important when selecting a vendor is key. We plan to seek a vendor that can handle a wide range of PCB types, materials, and complexities. This includes single-layer, multi-layer, rigid, flexible, and rigid-flex PCBs. For our project, we have been looking at multi-layer vendors since we have been looking at a 4-layer PCB since it is the most common, however, it will still not be as complex as PCBs that can be found throughout the industry. A good PCB vendor will provide a Design for Manufacturability (DFM) analysis to help optimize our design for efficiency and cost-effective manufacturing. They should be able to identify potential issues and suggest improvements before production of the circuit board begins, this is a key part for us as undergraduate students since we may be very prone to mistakes specially in PCB design even though we have striven to have it reviewed as much as possible before committing to the final design.

In the world of engineering QA or Quality Assurance is on the most undermined yet important aspects of succeeding in a project. The vendor should have a robust quality management system in place, such as ISO 9001 certification, which is mentioned in our standards to strive for in the design, to ensure that the PCBs meet the highest quality standards. They should also provide detailed inspection reports, including Automated Optical Inspection (AOI) and X-ray inspection results

which are key elements in the production line for Quality Assurance. Our PCB vendor should have a dedicated support team that can provide quick assistance with design-related problems and manufacturing issues. Fast Turnaround Time is a highly important characteristic as we have need to have the board for testing and troubleshooting in our system as quick as possible to exceed in our project. With this, expedited prototyping and production services are expected to help us meet the tight deadlines. Vendors may also have their own stock for parts that are needed in the PCB in case some parts are already out of the market even though we sought for parts that do not fall in this area of trouble.

5.3.1 OSH Park

OSH Park is a United States-based PCB vendor that is known for high-quality, lowcost PCB manufacturing services. They specialize in providing small-quantity orders for hobbyists, makers, and engineers, which is perfect for our senior design project.

OSH Park supports various PCB types, specializing in 4-layer and 2-layer boards. Some of the advantages that we found when researching this vendor were affordable pricing as OSH Park offers competitive pricing for 4-layer PCBs, making them an attractive choice for our small-scale projects with limited funding from Ocean-Insight. However, regarding the low-cost manufacturing, quality is not an issue with this vendor from what we see as they are known for delivering highquality boards, ensuring good performance and reliability for many designs.

They typically offer quick turnaround time service for 4-layer PCBs, which they estimate to be 9-14 days. It is especially beneficial for us for the previous mentioned reasons. OSH Park also has no minimum order and being students working on a project this is a key characteristic since we are not looking for a high-volume order as a company in the industry.

Their manufacturing facilities are also based in the United States, which is an advantage for easy communication with the vendor as well as shipping services and dates regarding the same. Their website seems to also be not highly complex to use as there is an option to simply drop the PCB files outputted from the design software to continue with the ordering.

Most of the disadvantages of OSH Park are mostly for big companies ordering highly complex designs and high volume which do not apply to us.

5.3.2 JLCPCB

JLCPCB, on the other hand, is a China-based PCB vendor also known for small to large scale production and manufacturing of PCBs internationally. They cater to various types of PCBs, based on their webpage, including 4-layer boards. JLCPCB

also seems to be great competition on prices since they seem to be cheap and based on layers and components per board.

JLCPCB has a large product volume capability which does not apply to us, but it is something highly sought for in the industry. They offer Surface Mount Technology (SMT) assembly services, providing a one-stop solution for customers who need both PCB manufacturing and assembly, all our components were selected to be SMD for the circuit board, so this is an essential feature to us.

Unlike OSH Park, us customers get better options for customizations of the board specifications, such as thickness, solder mask color, and surface finish, offering more flexibility in meeting project requirements, and creativeness. JLCPCB also provides a quick turnaround time for 4-layer PCBs. Regardless, some disadvantages may impact us. The main one being that they are a China-based company.

Being based in China, this vendor may have higher shipping costs and longer shipping times for customers like us that are in the Americas compared to local vendors such as OSH Park.

The issue of communication may also be a problem since while the service is provided in English, some language barriers may still be in place in the understanding between costumer and vendor, as well of time zone differences when seeking costumer support.

As we design our PCB with the selected software we seem to decide to go with OSH Park as their advantages apply to us even more as well as not applying to disadvantages with JLCPCB. However, we have be seeking to be quoted by both vendors to have a clearer view on what we should choose based on time and pricing.

6.0 Project Hardware and Software Design Details

The system overall is comprised of a great variation of subsystems that have their own specifications, functionalities, and tasks within the overall functioning of our project. Across the many sourced components only a couple are picked out to comprise each different subsystem, for the most part, the most critical and key components make up the need for a different subsystem. This is easily seen in the schematics that will be shown further ahead.

The PCB and its schematics were designed to serve a variety of purposes that derive from only a couple of inputs coming from the PC and power supply unit of 24V, as well as the aid of the MSP430EXPFR6989 which is the development board to program our microcontroller. Each subsystem has its own schematic for the

sake of simplicity as when we were studying the new software of Altium we learned that it is also the industry norm to categorize the schematics for organization which is a huge part of being an engineer.

6.1 Initial Design Architectures

Our design has two main subsystems that comprise the main functionality of the printed circuit board. The first subsystem is the humidity and temperature sensor logic. It includes the pull-up resistors, capacitors and required voltages as specified by the device's datasheet, the schematic, due to spacing matters, also contains the connector for the microcontroller schematic.

The second main subsystem is the safety system for the laser enclosure. This subsystem's main function is that of latching closed or letting open the door that gives access to the sampling kit and well plate reader as well as the laser. The reason for this implementation is for safety. The laser used in our project could be highly harmful to humans that may lead to blindness or burns. In this sense, a device that holds the door closed is a key component of the project for the user's protection when realizing the function of the system.

Supporting the main subsystems there are other smaller circuits that are essential to the proper functioning of the project. These "sub" subsystems are ones that communicate the main subsystems with external devices or aid communications from one side of the board to the other. A couple examples of these before we dive into them are the buck converters that determine the two 3.3V and 12V rails being used in the system as well as containing the main PSU connector from which these voltages are derived in their respective voltage regulators as seen in the buck converter voltage regulators section.

Another supporting system is the USB interface to communicate with the computer and send and receive the respective data such as sensor outputs on the



temperature and humidity values that are go into the MCU via I2C and are then

sent into the computer through this interface as well as the signals to turn on and off the fan based on the logic that will be used behind the obtained values. The interface is shown in the following PCB schematic.

This system shows the usage of connectors and various devices which purpose serve for the reliability and translation of signals coming from the computer via USB. The USB signals come in a differential pair which will be described shortly after negative and positive from the computer USB connector and fed into the PCB connector that land into the FT230XS-R which is a USB to UART converter.

The now UART protocol signals are received by the digital isolator SI8622EC-B-IS as RXD and TXD. The purpose of the SI8622EC is to as its description infers, digital isolator, to isolate the digital signal coming in from the overall signals within the PCB that are happening. Just like this component in the system, the USBLC6-2SC6 serves a very similar purpose. The USBLC6 is dedicated to the line protection of high-speed signals such as USB 2.0 which is what we have be receiving through the connector from the computer. The very low line capacitance of the device secures a high level of signal integrity without compromising in the case of ESD strikes. The MCU then receives the ultimately transformed RXD and TXD signal and reliable communicates with the computer.

Figure 58 - USB interface within PCB.

The concept of differential pairs is also a key factor in the reliability of the signal across this whole system even with all the protection devices and several details must be considered when using the differential pairs. They consist of two closely spaced, parallel traces that carry what are called complementary signals. These complementary signals are referred to as the positive (non-inverted) and negative (inverted) signals.

The differential pairs are implemented in our PCB design and many others dealing with highly sensitive signals as they provide noise immunity, as differential signaling is less susceptible to common-mode noise. The receiver then is only able to detect the difference in voltage between the two lines. If both traces are subjected to the same noise, it will not affect the differential signal, as it will be canceled out in the receiver. This technology also offers lower electromagnetic emissions. As the positive and negative signals in a differential pair are complementary, the magnetic fields in each other tend to cancel out, reducing the amount of electromagnetic radiation emitted by the traces.

To ensure the proper usage of differential pairs and the signal integrity, it is important to keep various details in PCB designing. It is essential to keep the trace lengths of the positive and negative signals as close as possible to minimize the timing effect between them. The positive and negative traces should be routed parallel to each other with minimal crossovers or changes in direction. This helps maintain the desired coupling and impedance control. For minimizing reflections and signal distortion, the use of smooth bends with angles greater than 90 degrees is essential when routing differential pairs. Vias should then, by common sense, not be used as it increases the risk of these details happening.

The next supporting system is the one ensuring we can have a way to program and debug our microcontroller, so it is possible for the whole PCB to properly follow its functionality. As small as it may seem this small subcircuit is the reason our project will hopefully work as intended. As shown in the MCU schematic, the SBWTDIO and SBWTCK which stand for input/output and clock pins from the microcontroller are connected into the connector that externally communicates with the MSP430EXPFR6989 Launchpad so that the USB interface within the development board can be used to program our microcontroller. These connections can be seen in the following schematic.



Figure 59 - Microcontroller connections and overall schematic.



Figure 60 - Spy-Bi-Wire connections for MSP430 programming.

A pull-up resistor and pull-down capacitor is then used to ensure the proper reliability of the connection between the launchpad and our microcontroller within

the PCB as specified in the MSP430FR6989 datasheet which also served as a guide to see all the connections. In the following image we can see where the connections will fall into the Launchpad.



Figure 61 - Jumper cases removed to disconnect the integrated microcontroller within the launchpad.

The image shows the jumper cases being taken out which disconnect the integrated microcontroller within the Launchpad to its programming pins. The female jumper cables are then connected into the SBWTDIO and SBWTCK and connected to the respective pins to connect with our microcontroller for its programming that will be done by the USB connecting with the computer that uses the Texas Instrument's CCS app for its programming.



The finished PCB is illustrated showing every subsystem, it is designed in a cascading way as power enters through the top left side and converts and distributes into 12V and 3V3 as it goes through many components down and right of the PCB. On the very bottom right corner is the isolated region for the USB communication with the PC powered by the same.

6.2 First Subsystem

The first main subsystem consists of the HIH6030-021-001 humidity and temperature sensor circuit. This circuit is based on the I2C communication with the microcontroller as this is the supported communication protocol for the sensor as per its datasheet. Within the device's documents it is also evident that some supporting passive components are also needed which will be pictured in its corresponding schematic along further explaining of the circuitry behind this subsystem and logic used.



Figure 62 - HIH6030-021-001 sensor connections and logic.

The datasheet for the sensor shows that two 2.2kOhms pull-up resistors are needed for the SCL and SDA lines to be connected into the microcontroller's designated SCL and SDA pins. Two capacitors are also to be put close to the sensor's power supply pins for decoupling and power reliability. The I2C connection will be fulfilled as the MCU is to be programmed to use this interface and convert the values then sent by the sensor as it reads the temperature and humidity around its environment.

The HIH6030-021-001 will also be responsible for the logic behind the fan circuit. The fan will be ON or OFF based on the values outputted by the sensor and the math the microcontroller will be programmed with, then giving the logic behind the

functioning of the DC fan. The circuit for the fan is also pictured on the right side of the schematic. The fan is controlled by a NPN transistor which controls the current flow of that side of the device to go to ground and the functioning of the same.

As shown in the schematic by the FAN_SIG port, a signal coming from the microcontroller goes into the 74LVC1G08GW,125. The 74LVC is a device by Nexperia that works as an AND gate. With distinction with regular logical AND gates, this device does not turn on for an input of 00, only for a 11 input. Which means that even if it is an AND gate the current will not pass for two low inputs coming from the microcontroller.

Based on the values from the fan the microcontroller will or will not send a current out of the respective GPIO pin to go into the AND gate. Since MCUs are known for outputting a small amount of current from the IO pins, the AND gate is used as a buffer. Connected to the 3.3V supply, the AND gate can amplify the current from the microcontroller when detecting an 11 input since its inputs are connected to the same pin, meaning the inputs will always be either 11 or 00, ON or OFF respectively. The reason behind this is to ensure that the NPN transistor has enough current at the gate to turn on and let current flow through from the collector to emitter hence turning ON the fan. The 100-ohm resistor is used for AND gate and microcontroller pin protection and the 4.9kOhm is used to amplify the voltage at the gate to at least 12V.

The MCU communicates with the sensor by requesting communication with the sensor using the 0x27 hexadecimal address which also starts the first measurement of temperature and humidity from the sensor. Then, on the second communication with the sensor by the MCU, the values are retrieved and obtained as 4 bytes of data of which 2 of those are respective to the temperature and humidity values we want. However, 2 bits of the 16 received for each are status bits therefore are sent through a data conversion within the code after being spliced into two. When these 2 bits are masked, and we obtain the final 14-bit value it goes through the given formula in the datasheet and the two different results are obtained and then sent through UART by the USB connection implemented.

6.3 Second Subsystem

The second subsystem of our hardware is the safety systems and related components. The star of the show in this section is the safety interlock. The safety interlock itself is operated by the contacts inside attached to a coil. This allows us to lock the enclosure of our spectroscope. The locking mechanism of the interlock is activated when we detect that the window is closed, and once the customer initiates the scanning. When this happens, the coil inside the safety interlock energizes, and locks the enclosure. This coil works at 24 volts DC, which is provided by the power supply that we have selected. Operating this coil effectively

requires another coil, given that our microcontroller and our other peripherals do not operate at 24 volts DC.

The secondary coil is in a relay that is on our PCB, with contacts for wiring going into the safety interlock. This relay separates the (relatively) high voltage of the safety interlock from our lower voltage microcontroller. The relay is wired by default in the normally closed position, not allowing any current to flow, and leaving the coil in the safety interlock turned off, allowing the window to be effectively unlocked. Upon using the spectroscope, the microcontroller will check first if the window is closed, if it is not closed, an error message will be presented to the person using the device that they need to close to window to continue operations. Upon closing the window, the monitor circuit in our safety interlock will be closed, meaning the signal to the microcontroller shows that it is closed. The microcontroller will then change the level on the GPIO that the safety interlock is connected to. This in turn will be connected to the base of a transistor, in parallel with a pull-down resistor. Once this happens, the collector current will flow into the relay on our PCB, energizing the coil inside the relay and switching the circuit to a closed position. Once this is done, the safety interlock will be activated due to current flowing in its coils, and the window will be locked. Only once these steps are done can the actual water analysis begin. Below we can see the electrical schematics of how the safety system works. One more thing to note here is the usage of the diode between the contacts on the coil. This diode is here for protection. When the relay gets disengaged, the coil that is inside is still energized. This means that the electrical power stored in the coil, which is essentially an inductor, wants to escape. This generates a potential difference which will then create a current that can go into our transistor which can damage it and damage the other components in our microcontrollers depending on the severity of it. This phenomenon is known as back EMF. The diode prevents this by only allowing current to go one way, it also dissipates this stored energy in the form of heat, allowing us to safely operate the relay without fear of damaging our other components. Below we have provided an image of this subsystem's schematic.



Figure 63 - Second subsystem schematic.

6.4 Software Design

The software involved with such a system is essentially what makes our machine work. The software will control essentially everything; the laser, the motor that moves the well-plate over the laser, and the spectrometer. The code will also oversee collecting the data, saving the data, translating the data, processing the data, displaying the GUI, displaying the data in the GUI in a way that means something to the user, and having customization options like manually setting the well plate, what communication port the laser, motor, and spectrometer are connected on the computer, etc.

Below is an example of the code that will take the data from the spectrometer and turn it into something that is easier to understand and can compute results from.

```
x = imread('SHS_Test.png').
F = fftshift(fft2(x))
imshow(mat2gray(log(1+abs(F))),'InitialMagnification',200).
```

The code above takes an image that was generated by the spectrometer reading the data received from shooting the laser into the sample in the cuvette on the wellplate, performs some calculations that include a Fourier's series shift, and then magnified and enhanced to make the image clearer and the spikes of the data more understandable and meaningful to us and the software. The dark image directly below is an example of the image generated by the spectrometer, also called "SHS_Test.png" in the code above.



Figure 64 - Imported interferogram ready for image processing (to undergo a 1D and 2D Fourier Transform).

After the next two lines of code that perform the calculations and image manipulations, we receive the image below. This does not mean much to us now but by analyzing the brightness of each point we can determine what contaminants are most prevalent in the sample.



Figure 65 - Resulting 2D Fourier Transform of the interferogram seen in figure 64.

The picture above shows a few bright spots in a horizontal line across the center of the page. Each of these spots can be related to the peaks in the IR spectrum seen below. Although the spectroscopy data below is chemistry related; the concept is still the same. The data provides insight as to what compounds are most prevalent in the sample.

The more prevalent the compound is in the sample, the larger the peak. The difference between the spectroscopy data below and the spectroscopy data above is that we are looking at them from different angles. The data above is looking at it from the bottom so instead of seeing large peaks we see bright lights.

The brighter the light is in the image, the stronger or taller that peak is, and therefore, means that the substance that is present in the sample and appears at that peak is more prevalent than others.



Figure 66 - Example of infrared spectrum plotted as transmittance versus wavenumber.

To be able to make the software capable of being used by someone wishing to operate the system we had to create a GUI that was capable of handling multiple inputs. The reason for this is that our system contains multiple major components which primarily include the spectrometer, the laser, and the motor. Below you can see an initial prototype for this GUI. There are a lot of features now, but they are suggestions given by industry professionals when asked what they like to see when using a spectrometer. Some of these buttons are stretch goals, some are unnecessary, and some are absolutely required to be there.

etup	+							
User Info Initialize Motor			Spectrometer Setup Clear Dark Spectrum Get Spectrum Spectrum Spectrum Pea	secs) Get k	Laser Setup Turn Emission ON Turn Emission OFF Shutter OPEN Shutter CLOSED	Lock Unlock		
Initia Moto Motor C	itialize Notor Notor Initialize not connected		not connected	Motor Setup Go To Start Current Position Current Position 1			Lon Lasu	
Laser C COM30	r OM # D ▼	Initialize UnInitialize	not connected	Toggle Absolute(m	v +			
Spec	trometer	Initialize UnInitialize	not connected	COM30 V Poll Temperature : Humidity :	Sensors 0 °C 0 %R	н		

Figure 67 - GUI Layout featuring a variety function that can control the motor, laser enable/disbable, and spectrometer/camera detection, including a useful message prompt.

Some of the more important functions above are in the initialization section. This section is responsible for connecting the components to the computer that will be running the software required to control our spectrometer.

To connect the laser and the motor to the computer, we must determine the correct COM port that is associated with the component. This can be done by pulling up the device manager for your computer and seeing which COM port appears when plugging the device in.

Once that is done, select the COM port from the drop-down menu and press the initialize button to "connect" to the part. The user will know when the part has been connected to the software because the "not connected" message will change to "connected". This process is the same for both the motor and the laser.

The spectrometer has a different hardware connection so simply pressing initialize is all that is needed to connect (assuming that the spectrometer is turned on and all the necessary hardware connections have been made).

Some other interesting commands that will be used in the GUI is the creation of positioning buttons for the motor. To maintain accurate results, it is sometimes necessary to reset the location of the well plate to ensure that the well-being scanned is the well that we desire.

For that reason, we have implemented a "start" and "center" button that will automatically go to the first well in the plate (or the "start") or the well that is halfway between the "start" and the "end" wells. This start and center will have a default setting, but these values can be edited by the user. The user will also be able to manually move the well plate if they desire a specific well be analyzed.

To fully understand how the code interacts with the components to bring our system to life; it is important to understand how and why our code was written the way that it was. Throughout the program there are lines of code that update the various writing to demonstrate updates to the setup and that the actions performed by the user are being processed or have been successfully (or unsuccessfully) completed.

Most of the communication will occur in the user info text box as this is the easiest way to clear and replace any messages that the user should know. Most messages are updates on the process the code is going through so that the user does not think there is a malfunction or code error. Examples of these intermediary messages will be provided later.

User Info				
Initialize Motor	Initialize Motor			
In iti - line				
Initialize				
Motor				
Motor COM #	Initialize	not connected		
COM30 v	UnInitialize	notociniotica		
Laser				
Laser COM #	Initialize	not connected		
COM30 =	UnInitialize	not connected		
	Initialize	not connected		
Spectrometer				

Figure 68 - Layout of initialization and message prompts.

To start, we have gone over the code for the user info and the initialization sections of the GUI. Initializing all 3 components of the system displayed in the GUI is indispensable and must be completed before any other actions are able to be completed. The reason for this is because the initialization is what connects the components to the software. Once that connection has been made, the user will be able to take control and perform the actions available to them. To complete the initialization the user must simply choose the COM port associated with the component and hit the "Initialize" button.

Once that has occurred, the user's responsibility has ended, and the program will take over. First, the code will display a message that the COM port has been set to the one chosen by the user and is attempting to make that connection. At the same time, the software will attempt to "open" that port which means that the communication port is allowing data packets to be sent through. The software will know that the port is opened when the port accepts the test packets that are sent through. After that has taken place, the software will set the baud rate, number of data bits, flow control, parity, and number of stop bits. The reason these must be set is to ensure that the communication between the two devices is smooth and does not result in any unwanted "collisions" that could compromise the data sent across and disrupt the integrity of our system. Once these parameters have been set, the two devices will be free to communicate, the buttons related to the initialized component will be enabled, and finally the text "not connected" will change to "connected". This process is essentially the same for both the laser and the motor.

However, the spectrometer does not have the same process of "connecting" to the computer. This is since the spectrometer is not actually connected to the computer and instead is connected to a camera that sends the pictures that it takes to the computer through USB. Furthermore, the spectrometer requires its own software to be downloaded and installed to the user's computer which will automatically be added to MATLAB as an extension. Once the extension has been added, the code will be able to call the various functions provided by the library. Unlike the motor and the laser, the spectrometer does not have a COM port since it is not directly connected to the computer. Instead, the code will call a wrapper class that searches for all available spectrometers. If none are found, the "User Info" section will display the message "No Spectrometers Found". Otherwise, the message "Found Spectrometer" will be displayed. Once the spectrometer has been found, the library will fetch the integration time, wavelength, and spectrum values from the spectrometer. These values will be used later in the actual calculation of the spectrum associated with the sample being analyzed.

Once the relevant code has completed running successfully, our motor, laser, and spectrometer will have been initialized and connected. Each successful connection enables that components "section" of the GUI.

Motor Setup				
		x	Y	
Go To Start	Current Position	1	1	
	Toggle Absolu	ute(mic	rosteps)	
		X		
		10 🔻	r 🔸	

Figure 69 - Motor setup layout; includes automated positioning features.

Arguably the most important section of the GUI is the motor. For this reason, it will have the most functionalities available to the user as there are so many possibilities that can occur that fall under the responsibility of the motor. The main ones are the use of moving the motor so that the bottom left well is directly over the laser (thus setting the motor at the "start". The same concept applies for the center (the center well will be placed above the laser). "Set New Start" and "Set New Center" buttons will be added but require the ability for the user to manually set the position of the motor. The ability to position the well plate as desired by manually setting the X and Y coordinates has not yet been implemented but will be added for the "Set New" features to be incorporated in the GUI. Both the manual positioning and the "Set New" features feature the

same process of overriding the values contained in the XstartAbsolute value with the X-Y coordinates that the motor is currently at. Nevertheless, accidents happen and as a safety measure in case the user accidentally sets a new start or center, the X-Y coordinates for the original start and center have been saved in the code and can easily be reinstated by simply pressing the "Reload Defaults" button. This button essentially restarts the motor without disconnecting it or moving it. Instead, the code will take all the variables that contain the values that can be set by the user and will overwrite them with the original values hardcoded in the Zaber Motion Library.

Spectrometer Setup		
Clear Dark Spectrum	Integration Time (secs)	
Get Spectrum	Set Get	
	Spectrum Peak	

Figure 70 - Spectrometer initialization and spectrum detection. Also includes a feature to remove baseline/dark-noise.

A common misunderstanding of the spectrometer is that the spectrometer itself is connected to the computer when it is initialized. However, the spectrometer is not connected to the computer directly, but instead, the camera that is connected to the spectrometer is connected to the computer through USB.

The camera will take pictures of what the spectrometer captures and transmits them to the user's computer over the USB cable. This spectrum is what is shown in the first image of this section and does not mean much to the user until the image has been run through more code to have the appropriate mathematical transformations performed on the values in that spectrum.

Once the spectrum has been saved, the user can hit the "Clear Dark Spectrum" button which sets all the pixels in the spectrum to zero. Setting all the pixels to zero essentially resets the spectrum that the camera was transmitting so that when the next well is analyzed, the spectrums will not overlap and provide the wrong data to the user.
Laser Setup	
Turn Emission ON	Lock
Turn Emission OFF	Unlock
Shutter OPEN	
Shutter CLOSED	
Laser OFF	Edit Laser

Figure 71 - Layout of laser control to enable/disable and control intensity.

The lases does not have many setup options for the user for a variety of reasons. For the most part, the laser cannot be changed. The wavelength, direction, and positioning of the laser is all fixed and part of intense calculations done by us to ensure that our system works as intended. Furthermore, the laser is a safety hazard as it is a powerful, concentrated source of high-energy electrons at a very high temperature that could easily be harmful to anything organic, including humans. Therefore, the laser set up features have been limited to turning the laser on and off, as well as how strong the laser is emitting. Finally, the edit laser button is available to edit the amount of voltage/strength of the laser as well as manually turning it on and off.

Due to the existence of a security system dedicated to safety from lasers, it was decided that the Lock and Unlock features of the safety system is included in the laser setup. The reason for this is that if the laser is on, the user should hit 'Lock' until the laser is turned off and they should then hit 'Unlock'. Locking prevents anyone from opening the latch to the well-plate which is where the laser is shooting directly up and out of the enclosure.

Temp Sensor COM# COM30 V	Poll Sensors
Temperature :	0 °C
Humidity :	0 %RH

Figure 72 - Layout of spectrometer and laser setup.

Another part of our system is the ability to poll the sensors for the current humidity and temperature inside the enclosure. Similarly, to the laser and motor, these are connected to the system and require the user to select a COM port to be able to effectively communicate with the sensors. The sensors operate based on serial commands to communicate with the software. The sensors allow for live updates with the click of a button. For more information about the sensors, refer to Section 3.4.3 Temperature & Humidity Sensor Components.

Spectrometer	Setup		Laser Setup		
Clear Dark Spectrum Integration		ne (secs)	Turn Emission ON	Lock	
Get Spectrum	Set	Get	Turn Emission OFF	Unlock	
	Spectrum F	Peak	Shutter OPEN		****
			Shutter CLOSED		
			Laser OFF	Edit Laser	
Go To Start Curr	Igle Absolute	1 1 (microstep x) v +	ps)		
Temp Sensor COM#					
COM30 v	<u> </u>	Poll Sensors			
Temperature :		0	C		
Uumiditu		0	N DH		

Figure 73 - Layout of spectrometer and laser setup.

Once the user has connected to all the components and have set up the system to their liking, they can begin running the system and being to receive an analysis of the samples on the well plate. Once this has begun to occur, the user can hit the "Get Spectrum" button. At this point, the software will capture the Raman signals from the laser and captured by the spectrometer, process the matrices and data within the image taken, and uploads it as a graph in the white box on the bottom right.

These sections of the GUI are the main portion of the system. Without these sections, it would be impossible to modify the system at all, making it much harder to operate the system anyway other than the default setup. In the future, attempts at automating these features in the code to preserve the integrity of the system and make the system much more foolproof will be implemented.

6.4.1 Supplemental Software

When the user connects their computer to our spectrometer to run the associated software there are a few supplemental software that must be installed on the user

computer to successfully execute the program. Not only does the program connect to our components to tell the system what to do and when, but some of the settings for those components can be edited before starting the analysis of the system. Therefore, to edit the settings for the machine, some commands must be executed to communicate those settings or preferences to the associated component. Most of these additional libraries are generally downloaded along with the main MATLAB program files during the initial MATLAB installation. However, the motor requires an extra installation.

To operate the motor (which includes, moving, resetting, connecting, initializing, and any other operations performed by the motor) the user must install some additional software. The motor is a Zaber motor which requires a library that contains all the commands needed for the motor to perform any operation. The commands must be written in the MATLAB code but to compile the commands, the Zaber Motion Library must be installed and added to MATLAB as an extension. This extension can be found by going to the Zaber website and it will automatically be added to MATLAB once it is installed. It is a relatively small installation with a file size of less than 1 Gb. Once the library has been added as an extension, MATLAB will be able to recognize the commands for the motor thus allowing the user to perform any of the operations available ono the GUI.

Similarly, the spectrometer also has its own software. Since it has its own means of connection and transmits data instead of working as a moving part like the motor and laser, it needs its own set of commands and tools to operate as expected. Therefore, the Image Acquisition Toolbox for the iDS Camera is required to be added to MATLAB. This will allow the camera that is going to be used in conjunction with the spectrometer and transmit the images generated by the spectrometer when analyzing one of the samples. For the camera to be able to communicate with the spectrometer it must be able to use the libraries in the toolbox. Once the toolbox has been downloaded, it will be automatically added as an extension to MATLAB. Doing so allows for the camera to have access to the library and perform its tasks accurately by relaying the images produced by the spectrometer back to the user for further calculations and analysis.

One thing that is inevitable when it comes to programming is that new, upgraded versions will come out overtime. The run time used to develop this software was MATLAB Runtime version 9.6. When the user downloads MATLAB there could potentially be a newer version that was released after the time the spectrometer's code was developed. Unfortunately, MATLAB is not backwards compatible so programs developed under an older MATLAB compiler version will not run on newer MATLAB compiler versions. The easy way to fix this program is to install the runtime that was used to develop the program. In this case, our system uses a program developed on MATLAB runtime version 9.6, but this can also be determined by simply attempting to run the program. When the code tries to execute, the user will be met with an error stating that MATLAB runtime version

9.6 was not detected on the computer. Once the appropriate MATLAB runtime version is added to the directory containing all the MATLAB files, the program will execute correctly automatically.

6.4.2 PCB Design Software

Modern PCB design, as well as trouble shooting, is primarily done through software. Many tools are available web or application-based with licenses offered that can be hundreds of dollars. Electronic Design Automation (EDA) or Computer-Aided Design (CAD) tools, provide a wide range of features that assist electrical engineers throughout this design process. Printed circuit board design software allows engineers to create and edit circuit schematics, which represent the components, communications, and connections within a circuit. Schematic capture, a process widely integrated in many PCB design software's, helps in defining the logic behind a circuit and organization of the PCB components before moving on to the layout phase.

All EDA tools come with extensive libraries of components, that may include symbols, also referred to as designators, for easy component representation in a schematic as well as to-scale footprints for PCB layout. These libraries can be customized and expanded by downloading external libraries or creating a user's own to include new or specialized components, saving time and ensuring consistency and automation across designs. Design Rule Checking (DRC) is another very popular feature that can perform automated design rule checks to identify errors, such as incorrect trace spacing, overlapping pads, or insufficient clearance between components. This feature aids in identifying issues early in the design process that have to do with layout and board spacing, reducing the likelihood of an issue happening with supplier, manufacturing problems and expensive revisions.

CAD tools enable designers to create and optimize the physical layout of the PCB, including component placement, trace routing, and copper pour areas. Advanced routing features, such as auto routing, can aid in the time constraint of routing traces and speed up the design process along improving the overall quality of the final product. 3D Visualization: Modern PCB design tools offer 3D visualization capabilities, allowing designers to view their boards in a 3D environment, by selecting components, cross checking with schematics, and even verifying tracing all while showing a to-scale 3D model with color. On that same hand, this feature may aid in identifying potential mechanical interference, optimizing component placement, and verifying clearances.

Collaboration and quality assurance are the most undermined yet most important factors in maintaining a healthy project outlook when working with a group of engineers and even suppliers involved in the manufacturing of the PCB. Many CAD and EDA tools now support collaboration features, enabling multiple

designers to work together on a single project. This can include version control, file sharing, and real-time communication tools, helping to maintain the design process across engineers, ensure consistency, and aid in quality revisions. This software can generate a variety of useful electrical manufacturing files, such as Gerber files, and assembly drawings based on the project. These files are required by fabricators for the proper manufacturing and assembling of the PCB, ensuring compatibility with the desired functionality of the board and processes and equipment used in the manufacturing environment.

6.4.2.1 Altium

Altium Designer is a highly powerful and comprehensive PCB design software developed by Altium Limited. It is one of the most popular software's used by professionals and large organizations in the electrical & computer engineering industry for designing printed circuit boards. Altium encapsulates all the key features described in the previous section, with the most resalting one being the highly accurate and interactive 3D model, as well as Altium Viewer which is a feature mostly unique to it in the PCB software market. Altium Viewer lets you drop a zipped folder that is outputted when the project is finalized in its actual application into a web-based "viewer" site. The site will take all the files that contain Gerber, schematics, drawings, even 3D model and let you view them for free and even interact with the features.

The cost for a license of Altium Designer, however, is on the higher side for most of the software's in this market. This price markup is reasoned to be accurate as Altium is arguably the most popular application used for PCB design in the corporate world. The price is around \$7,000, with an additional annual subscription fee for maintenance and support. Many other options are given, however. The use of monthly subscriptions, free trials, and even free student licenses are also great options for obtaining this high-end software. Luckily, as University of Central Florida students, we were able to get a hold of Altium's free student license that runs a little until after graduation and will be using it for our project PCB design.

Using Altium Designer will be a challenge as it has a steeper learning curve than most other software's of its nature due to its advanced capabilities and the many features integrated within its environment. However, Altium also offers a free introductory course for students to get kickstarted with the many features the applications have and a walkthrough project that will be of big help when realizing our own senior design project. It is primarily targeted at professional users and organizations with complex PCB design requirements, which plays a huge role in being our software choice.

6.4.2.2 EAGLE

EAGLE (Easily Applicable Graphical Layout Editor) is a popular PCB design software by Autodesk. EAGLE is known for its user-friendly interface and broad set of features, making it an attractive choice for beginners and professionals alike, in contrast to Altium. The software also shares most of the key elements that are looked for in a PCB software design application. In the University of Central Florida, we were first introduced to the application in EEL3926L Junior Design to design the Rangefinder project and be introduced into features such as schematic building, tracing, layout, and BOM tools.

EAGLE is significantly more accessible to Altium as their prices are reduced by around 5-10 times as much. EAGLE's user-friendly interface and available resources, such as tutorials and community forums, make it accessible to users with varying experience levels which is also attractive for us, but we may take on the challenge with Altium Design. The student license also seems to not have as many features. Regardless, Autodesk EAGLE is a perfect second option for us when it comes to realizing our PCB design for further manufacturing and will be falling into it if we run into challenges with Altium.

6.4.3 Microcontroller Programming

Microcontroller programming is an essential characteristic of embedded systems development, which enables control and interaction between various components within a device and enabling their respective functionalities. Microcontrollers are small, integrated circuits that convey a processor, memory, and a variety of input/output (I/O) pin elements. They are widely used in modern electronic systems and can be found in most of applications in the industry, from consumer electronics to industrial automation and medical devices. Programming a microcontroller involves writing code that manipulates the microcontroller's operations and manages its interactions with other components in the system, in this way, managing the operations of the whole system. A microcontroller, often referred to also as an MCU, can be identified as the engine driving a device. The code can be written in many popular programming languages such as C, C++, or assembly language.

C, C++, and assembly, the previously mentioned languages, are the most common languages in microcontroller programming due to their efficiency, and ability to have control over hardware. Microcontrollers typically have limited processing power and memory resources compared to normal computers. These programming languages are easily compiled languages that generate efficient machine code, allowing programs to run quickly and use minimal memory making them the first choice for MCU programming. C and C++, provide an easy and simple feature of manipulating the controls over the hardware, enabling developers like us to directly make use of memory, registers, and I/O interfaces, in this way, they are portable languages, which refers to the code written in these languages being able to be easily adapted to run on different microcontroller architectures with minimal modifications. To facilitate the programming, developers often use specialized software tools known as integrated development environments (IDEs) or programming software. These tools provide features like code editing, compilation, debugging, and flashing, streamlining the development process. We have a couple options to use in our senior design project as we immerse ourselves in MCU programming. Our primary choices are STM32 and CCS by TI. The reason for these is that STM32 are widely used in the industry and very versatile at the time of programming, CCS on the other hand is a tool that we were already introduced to when taking classes such as C programming and Embedded Systems.

6.4.3.1 CCS

Texas Instruments' Code Composer Studio (CCS) is one of the IDEs mentioned in the last section. The purpose of this software is to aid in the design and programming of the Texas Instruments' microcontrollers. CCS has been introduced to us Electrical and Computer engineering department students in classes such as Embedded Systems, EEL4742C. In this class we learned the concepts of embedded programming such as clocking, syntax, libraries, communications protocols, and therefore the use of microcontrollers. The lab challenged us to do difficult tasks with the MSP430 development board which used CCS for its programming through a USB connection to our computers. Concepts like interrupts, UART, I2C, SPI protocols were used in realizing many experiments with the board.

For this project we have be programming the individual chip, however. This chip will go into our printed circuit board to control the functionality of the project. However, to program this individual chip we have still need the TI development board used in class. Our abilities gained in this class will play a substantial role if we decide to go with Texas Instruments as the manufacturers of the MCU used in the project. On that note CCS has many features that will come in handy in the development of the project.

CCS has support for multiple programming languages, such as C, C++, and assembly, however, C language will be used in the programming due to our experience using it for many classes in the engineering department. TI has many forums and built-in features that provide us with generated code specialized for programming our microcontroller. This code ranges from startup code to building blocks essential for communication protocol formats. The debugging capabilities of CCS are key to us as undergraduate students as it is quick to not just detect,

but guide through error codes to improve our code. Code editing is a very popular feature that is one of the reasons for developers to pick and choose between IDEs and this software does not fall behind on that aspect.

The process of creating our program is simple not only because of our experience but also the nature of the IDE, CCS provides a comprehensive environment by simplifying the process of writing, compiling, and debugging code for TI microcontrollers such as the MSP430. Users can create a new project by selecting the target microcontroller and configuring its settings to their liking based on the requirements of the project. CCS then generates a project base with the necessary file. Once the code is written, it can be compiled and debugged using the built-in debugger. When the code is ready for deployment, users can flash it onto the microcontroller directly from the IDE with the use of USB that in our case may go from the development kit board MSP430 to our chosen individual microcontroller unit. This may be using wires and a breadboard, soldering or a specialized perf board for the chip we select.

6.4.3.2 STMCubeProg

STMCubeProg is another microcontroller programming software developed by STMicroelectronics for their own MCUs. This IDE contains a variety of tools such as libraries, for the development of STM32s. In contrast to TI's Code Composer Studio, they have very similar capabilities and features. Extensive libraries, multiple programming languages being supported as well as generated code to start up a project for simplicity and formatting.

Users can create a new project using the STM32CubeMX graphical configuration tool, which enables easy setup of microcontroller pins functionality and generates initialization code. We could then be able to write our application code using the preferred development environment.

Once the code is ready, it can be compiled and loaded into STM32CubeProg. The software provides debugging and tracing capabilities, allowing users to monitor and control the execution of their code on the target microcontroller.

When the code is fully debugged, troubleshooted and optimized, it can be sent onto the microcontroller using the supported programming interfaces. The differences are not very critical in this matter, but when there are they seem to lean into TI's CCS as the better capabilities of STMCubeProg do not apply to us. So, the matter falls more into which microcontroller is selected and then the corresponding IDE will be used.

6.4.3.3 JTAG & Spy-Bi-Wire

Spy-bi-wire by Texas Instruments is a 2-wire interface designed for programming and debugging microcontrollers, specifically for the MSP430 series microcontrollers that will be appearing in our project in the printed circuit board as the MSP430FR6989. The interface is comprised of two signal lines: the bidirectional data line, called SBWTDIO that is used for transmitting and receiving data, and the clock line, called SBWTCK, which synchronizes the data transmission between the host and the microcontroller.

SBW works by using a synchronous serial communication protocol where the host sends commands to the microcontroller by toggling the SBWTCK line while transmitting data on the SBWTDIO line. The microcontroller accepts this command by sending a response on the SBWTDIO line. This interface enables efficient access to the microcontroller's internal hardware, allowing for programming and debugging with minimal pin usage, a feature that is attractive for the PCB design. The SBW interface is the interface that we have use in our design to program the microcontroller as we are using a TI MSP430 device. The way it will be implemented also consists of using an MSP430 launchpad that has already been acquired. The Launchpad has an integrated USB interface that connects with a computer and is compatible with the SBW interface. This means that in a way, it is possible to program the microcontroller via USB. The jumper case will be removed from the SBWTCK and SBWTDIO that connects the Launchpad's integrated MCU and the communications side of the board. A female-male or female-female jumper wire will be connected to these two pins which at the other side will connect to our integrated microcontroller in our own printed circuit board into the same SBWTCK and SBWTDIO pins. From there we can connect the Launchpad to the computer via USB connection and the programming software will be able to upload and debug our microcontroller as needed.

On the other hand, the JTAG (Joint Test Action Group) interface is a standardized interface widely used for programming and debugging microcontrollers, ASICs, FPGAs, and other digital devices. It is very similar to Spy-Bi-Wire interface with the main difference being that it consists of a 4-wire interface. This interface includes the TDI (Test Data In) serial data input line, TDO (Test Data Out) serial data output line, TMS (Test Mode Select) mode selection line for controlling the state machine, and TCK (Test Clock) clock line for synchronizing data transmission between the host and the microcontroller. JTAG operates by implementing a state machine that allows the host to control the microcontroller's internal hardware. By manipulating the TMS and TCK lines, the host can issue commands and transfer data through the TDI and TDO lines. A great feature of this interface is supporting daisy-chaining between multiple other devices which makes mass production much simpler, but for our project it is not something useful.

The main difference between Spy-bi-wire and JTAG is that SBW requires only two pins (SBWTDIO and SBWTCK), making it more suitable for our device for simplicity and limited I/O pins and JTAG uses four pins (TDI, TDO, TMS, and TCK). JTAG is a versatile standard that supports a wide range of devices, including microcontrollers, ASICs, and FPGAs. JTAG would have been our choice of interface, however, if we had chosen an STM microcontroller as this is the format to do so in the industry. Spy-bi-wire is specifically designed for MSP430 series microcontrollers by Texas Instruments and hence picked out for our design for simplicity and device selection as JTAG has a more complex protocol and state machine compared to SBW.

6.4.4 TI Webench

TI, Texas Instruments, is a global semiconductor company that designs, manufactures, and sells a broad range of electronic devices and integrated circuits. It specializes in areas such as digital signal processing, embedded processing, and power management. We utilize their products a lot throughout UCF as their microcontrollers are key for embedded systems class as well as TI webench which is the feature we use in this project.

TI Webench is a set of online tools developed by TI that enable engineers to design, simulate, and create custom power supplies quickly and efficiently. This platform provides a highly intuitive user interface and a vast library of components, making it a great resource for a great scope of people. We used webench in senior design to make use of buck converters for our main power supply and step down the voltage to the steps that we needed throughout the system.

In this software users can input their desired specifications, ranging from voltage ratings, current ratings and the tool will generate a list of potential designs to meet those requirements. Then, these designs can be compared based on factors like efficiency, cost, and size.

After these simulated steps, engineers can step up to modify the designs to better suit the specific needs of their respective project, adjusting parameters such as input/output voltages, load current, and operating frequency for every single component that was placed at first by the tool.

On top of this, webench allows users to run simulations on their designs, testing performance under different conditions and identifying potential issues before placing into the desired schematic or building the physical model. A bill of materials is generated along with the design that shows the manufacturer characteristics, prices, and stock options for the selected components, as well as offering other alternatives in case it is not up to the engineer's standards. To finalize the development tool, TI offers the option to export the design instead of having to build the made circuit component by component by CAD design that can be put

into the PCB software of choice. It was a greatly helpful tool that was introduced to us in junior design and was the reason for our buck converter selection among other supporting components that aid the power distribution in the system.

6.5 Summary of Design

The design of the spectroscope can be broken into multiple different parts. The parts are the laser alongside the associated lenses and diffractors, the capture system and the processing computer, the temperature and humidity sensors inside the enclosure, and the safety systems that allow us to lock the enclosure as needed. The lasers hit the sample and then through Raman scattering we can detect the changes in the inelastic scattering. These changes are detected by the capture device that we have and is then fed into the computer system. The software on the computer uses fast Fourier transforms to then give us useful data in the form of wavelength energy graphs.

The temperature and humidity sensors inside the enclosure are used for ensuring that we have a consistent area for the spectroscope, since humidity and temperature both influence light scattering. The safety systems are there because we are dealing with high power lasers that can cause injury. The safety systems will lock our enclosure to ensure that nobody opens it during operation, as this can also be a liability to the company in case someone gets hurt.

7.0 Administrative Content

In this section we have discuss our bill of materials and finance. This section will also provide an organizational chart of the members of the team describing visually who they are, what their general responsibilities entail, and what their overall contribution to the project is to ensure successful completion.

7.1 Bill of Materials

This BOM is the summary of all the components to be used in the manufacturing of the printed circuit board to support our overall design. It showcases the designators tied to every single part as well as the quantity per and price total based on the selected manufacturer.

This BOM was exported from the finalized schematics in Altium by using the report manager feature and adding supplier links to all the different components to check for stock and market availability.

Name	Designator	Quantity	Cost per Part	
GRM21BR61H106KE43K	C1, C8, C12	3	0.258	
CC0805KPX7R9BB104	C2, C3, C7, C9, C10, C15, C16, C17, C18, C19, C21, C22, C23, C24, C25	15	0.31119	
C0402C470J5GAC7411	C4, C13, C14, C26	4	0.21	
GRM31CR61C476ME44K	C5, C11	2	1.56	
CL21B224KAFNNNE	C6	1	0.0854	
GRM1885C1H222JA01J	C20	1	0.0874	
USBLC6-2SC6	D1	1	0.23	
SML-LX0603YW-TR	D2	1	0.2768	
SML-LX0603GW-TR	D3	1	0.038	
RF302LAM2STR	D4	1	0.7	
MI1206K601R-10	FB1	1	0.154	
1734035-4	J1	1	0.7284	
3-794636-4	J2, J3	2	0.834	
1969795-1	J4, J?	2	1.25	
SDR1307-5R6ML	L1	1	1.09	
SDR1307-120ML	L2	1	0.95722	
BC817-25-QR	Q1	1	0.17	
EMX26T2R	Q2	1	0.53	
CRCW080530K9FKEA	R1	1	0.005	
ERJ-6ENF1002V	R2, R6, R10, R17	4	0.04	
ERJ-6GEYJ222V	R3, R4	2	0.018	
ERA3AEB1403V	R5	1	0.3163	
CRCW1206100KJNEA	R7	1	0.1	
RK73B2BTTD270J	R8, R9	2	0.2	
RC1206JR-07750RL	R11, R12	2	0.15	
ERA8AEB473V	R13	1	0.635	
CRCW0402100RFKED	R14	1	0.002	
RK73H2ATTD4991F	R15	1	0.089	
CRCW08051K00FKEA	R16	1	0.003	
MSP430FR6989IPZ	U1	1	12.8	
TPS563300DRLR	U2, U8	2	3.26	
HIH6030-021-001	U3	1	12.35	
FT230XS-R	U5	1	2.26	
Si8622EC-B-IS	U6	1	3.03	
74LVC1G08GW,125	U7	1	0.0453	
G5V-1-DC3	U9	1	2.03	
TOTAL:			46.8	

Table 16 - PCB Bill of Materials.

The components to be used in the printed circuit board were sourced for a balance in both performance and price which was a successful task as \$47 does not feel like a great amount for the functionality that out PCB will be performing in our project and the quality of the sourced parts.

7.2 Finance

This project has been financially sponsored by Ocean Insight in the hopes of the completed project having the required functionality and perform in the market. Many meetings have been done with the Ocean Insight team to analyze the specifications for the system as well as peer reviewing of the progress in our designs.

The bill of materials for the PCB will be given to the company as well as the green light for ordering the through a manufacturer as the one that were listed in this paper. The many optical systems within the design are also provided by Ocean Insight.

7.3 Team Organization

The members of our team are Juan Restrepo Diaz, Gibran Khalil, Julia Smith-Blanchard, George McDonald, and Sebastien Jouhaud. Our overall system contains many components and requires in-depth communication throughout the semester and a general understanding of all elements and components involved.

To truly enhance the overall system, we were compelled to understand it in a multidisciplinary fashion. For example, to properly develop a thermal/humidity sensor, one would need to understand the impact upon the optical components and therefore the impact upon the spectral information presented. The optical engineers would need to recognize the limitations of the motor performance in automation of well-plate movement and cuvette position to determine the optimal Raman probe position.

Even though there is an innate need for cross-discipline understanding, there was a general focus for each member of the team to ensure proper completion of the design and assembly. The responsibilities for each member of the team and their overall focus are described in the visual team organization chart.

Electrical Engineers Responsibilities					
	PCB Design and Assembly				
Juan Restrepo Diaz	Power supply design				
	Research in humidity and thermal impact				
	System integration between spectrometer, PCB, and software				
	Precision motor design and selection				
Gibran Khalil	Power supply design				
	Safety Systems design				
Optical Engineers	Responsibilities				
	Investigate imaging techniques				
Julia Smith Blanchard	Lens design				
	Contaminant research and selection				
	Spectrometer assembly and design				
	Illumination system design				
George McDonald	Spectrometer assembly and design				

	SHS modeling and simulation			
	spec			
Software Engineer	Responsibilities			
Sebastien Jouhaud	Spectral analysis			
	Spectrometer research			
	C++, MATLAB, Serial commands			
	Software integration and communication with various devices			

8.0 Conclusion

W.A.R.S. is an ongoing project through the summer semester of 2023 at UCF. It is advancing quickly and is well on track to being completed by the end of Senior Design 2. After much deliberation, the W.A.R.S. team has determined a list of parts and technologies that we believe will create the cheapest yet most efficient and reliable Raman spectrometer on the market. It is versatile, user-friendly, and has already begun to show promise as a series of individual parts that work as expected.

Now, the biggest difficulty for the project from a software perspective is finding a way to make the software run easily without having a bunch of hoops for the user to jump through. Ideally, an executable will be created for the user to run with just the click of a button, or the entire project can be put on a flash drive and the user will simply run a bash file that will automate all the downloads and extensions needed. From a hardware perspective, the largest obstacle is to be able to organize the hardware in a way that will not hinder the organization of any other components.

W.A.R.S has been able to come by a spectrometer prototype, motor, enclosure, various power supplies, and the various cables or other smaller materials needed to complete our system. The largest wait time will be the smaller, more delicate components of our spectrometer as well as the PCB's that first requires, we have all the parts before we can determine whether to build the PCBs ourselves or send them off to be developed by a 3rd-party manufacturer.

The team behind this project has dedicated themselves to creating the best possible machine with the time given. We strive to create a spectrometer that will produce accurate, reliable, and useful results to make the world a healthier place.

Appendix A: References

- Agency, E. P. (2023, February 14). *Drinking Water Regulations and Contaminants*. From EPA: https://www.epa.gov/sdwa/drinking-water-regulations-and-contaminants
- AMD. (n.d.). AMD Ryzen[™] Threadripper[™] PRO 5000 WX-Series Processors. (AMD) Retrieved March 22, 2023 from https://www.amd.com/en/processors/ryzenthreadripper-pro
- Arcing. (2021, December 28). (Safeopedia) Retrieved March 23, 2023 from https://www.safeopedia.com/definition/7641/arcing#:~:text=Safeopedia%20Explai ns%20Arcing-,What%20Does%20Arcing%20Mean%3F,to%20anyone%20expos ed%20to%20it
- Banerjee, S. &. (2004). Sample compartment temperature control in UV/Visible spectrophotometers. *American Laboratory, 36*(18).
- Cisco. (n.d.). What Is a LAN? (Cisco) Retrieved March 23, 2023 from https://www.cisco.com/c/en/us/products/switches/what-is-a-lan-local-areanetwork.html
- Crucial. (n.d.). *What is Computer Memory (RAM) and What Does It Do?* (Micron) Retrieved March 3, 2023 from https://www.crucial.com/articles/aboutmemory/support-what-does-computer-memory-do
- *Generic Standard on Printed Board Design*. (2003, May). (IPC) Retrieved March 24, 2023 from https://www.ipc.org/TOC/IPC-2221A.pdf
- How Much Does A Gas Chromatograph Cost? (2022, May 6). (Axion Labs) From https://axionlabs.com/chromatography-training/how-much-does-a-gaschromatograph-cost/
- Hymel, S. (n.d.). Getting Started with STM32 Introduction to STM32CubeIDE. maker.io.
- IEEE. (2018, August 31). *IEEE Standard for Ethernet*. (IEEE) Retrieved March 23, 2023 from https://standards.ieee.org/ieee/802.3/7071/
- IEEE. (2022, April 1). *IEEE Standard for DC Power Transmission and Communication to DC Loads*. (IEEE) Retrieved March 23, 2023
- Instruments, T. (2021). *Code Composer Studio (CCS) User's Guide.* Texas Instruments. Intel. (n.d.). *Intel.* (Intel) Retrieved March 22, 2023 from
 - https://ark.intel.com/content/www/us/en/ark/products/226453/intel-core-i51230uprocessor-12m-cache-up-to-4-40-ghz.html

- Intel. (n.d.). *Intel*® *Xeon*® *Processor E5450*. (Intel) Retrieved March 22, 2023 from https://www.intel.com/content/www/us/en/products/sku/33083/intel-xeonprocessor-e5450-12m-cache-3-00-ghz-1333-mhz-fsb/specifications.html
- Legaspi, E. P. (2020). UART: A Hardware Communication Protocol Understanding Universal Asynchronous Receiver/Transmitter. *Analog Dialogue, 54*.
- MATLAB. (n.d.). *MATLAB and Simulink Requirements*. (The MathWorks, Inc.) Retrieved March 22, 2023 from https://www.mathworks.com/support/requirements/matlabsystem-requirements.html
- McMaster, &. M. (1998). GC/MS : a practical user's guide. Wiley.
- Moglix. (n.d.). *Everything about RAM: Factors to consider before buying*. (MOGLI LABS) Retrieved March 3, 2023 from https://www.moglix.com/articles/everything-aboutram-factors-to-consider-before-buying
- Moran, M. J. (1986-99). National Synthesis on Volatile Organic Compounds (National Water-Quality Assessment Program), & Geological Survey (U.S. In *ccurrence and Status of Volatile Organic Compounds in Ground Water from Rural, Untreated, Self-Supplied Domestic Wells in the United States* (p. 15 (p. 3)).
 Rapid City, SD: U.S. Geological Survey, Information Services .
- Nana, E. T. (2019). Designing with I2C-Bus Devices. NXP.
- Prevention, C. f. (2022, May 16). Water treatment. From

https://www.cdc.gov/healthywater/drinking/public/water_treatment.html

Propagation Delay and Its Relationship to Maximum Cable Length. (2019, July 22). (LiveAction) Retrieved March 23, 2023 from

https://www.liveaction.com/resources/blog/propagation-delay/

Spangenberg, M. B. (2021). Ultraviolet absorption of contaminants in water. . *Sci Rep 11*.

Standardization, I. O. (n.d.). *ISO 9001:2015 Quality Management Systems -Requirements*. From https://www.iso.org/standard/62085.html

- The PyCoach. (2022, August 28). *Is a Mac or Windows PC Better for Programming?* (Medium) Retrieved March 23, 2023 from https://medium.com/geekculture/is-amac-or-windows-pc-better-for-programmingd5556bf06f1#:~:text=The%20Operating%20System%3A%20macOS%20vs,serv
 - ers%20are%20based%20on%20Unix.
- Tom Brant. (2022, August 26). *SSD vs. HDD: What's the Difference?* (PC Mag) Retrieved March 3, 2023 from https://www.pcmag.com/news/ssd-vs-hdd-whatsthe-difference

Appendix B: Copyright Permissions I. Image Permissions

UART IMAGE

From: Juan Restrepo Diaz <<u>juanfeliperd@Knights.ucf.edu</u>> Sent: Monday, April 24, 2023 10:26 AM To: Pena, Eric <<u>Eric.Pena@analog.com</u>> Subject: RE: Website image permission

[External]

Hi Eric,

Forgot to plug in the website link. https://www.analog.com/en/analog-dialogue/articles/uart-a-hardware-communication-protocol.html

Thank you! Juan

From: Juan Restrepo Diaz Sent: Sunday, April 23, 2023 10:24 PM To: eric.pena@analog.com Subject: Website image permission

Hi!

My name is Juan Restrepo from the University of Central Florida, and I am a senior in electrical engineering. I am working on a project for my Senior Design class along with teammates and doing our research we would like to ask for your permission to use Figure 2 depicting the UART connections functionality drawing. I would like to emphasize that your site, Analog, as well as your name, will be properly referenced and of great help! If there is anything else you need, please let me know.

Thank you, Juan

From: Laznik, Anna <<u>Anna.Laznik@analog.com</u>>
Sent: Monday, April 24, 2023 10:27 PM
To: Pena, Eric <<u>Eric.Pena@analog.com</u>>; Siegel, Bernhard <<u>Bernhard.Siegel@analog.com</u>>;
Cc: Legaspi, Mary <<u>Mary.Legaspi@analog.com</u>>; Juan Restrepo Diaz <<u>juanfeliperd@Knights.ucf.edu</u>>
Subject: RE: Website image permission

Hello Juan, Eric,

I see no issue with borrowing the image and including the appropriate reference back to the article/website.

Best regards, Anna

Anna Laznik Marketing Communications Technical Articles/Analog Dialogue

 Office
 (339) 645-3051

 Mobile
 (781) 619-4497

 Web
 analog.com





SPI IMAGE

------ Original Message ------From: Juan Restrepo Diaz [juanfeliperd@knights.ucf.edu] Sent: 4/23/2023 7:17 PM To: support@corelis.com Subject: Website image permission

External Email: Be mindful of links/attachments

Hi!

My name is Juan Restrepo from the University of Central Florida and I am a senior in electrical engineering. I am working on a project for my Senior Design class along with teammates and doing our research we would like to ask for your permission to use Figure 1 depicting the SPI functionality drawing. I would like to emphasize that your site, Corelis, will be properly referenced and of great help! If there is anything else you need, please let me know.

Thank you,

Juan



Copyright © 2022 Corelis, Inc. All rights reserved. Corelis, the Corelis logo, and ScanExpress are trademarks of Corelis, Inc. All other company and product names may be trade names, trademarks, or registered trademarks of the respective owners with which they are associated. Features, pricing, availability, and specifications are subject to change without notice.

C	support@corelis.com	$ \bigcirc \qquad \bigcirc \qquad Reply \qquad & & & Reply \qquad All \qquad \rightarrow \qquad Reply \qquad Reply \qquad All \qquad \qquad \qquad \qquad Reply \qquad$	\rightarrow Forward	Û	ŀ		
3	To Juan Restrepo Diaz				Mon 4/24/	2023 12:	:19

1

(i) Click here to download pictures. To help protect your privacy, Outlook prevented automatic download of some pictures in this message.

Hey Juan,

You should be fine to use the image, as our website is open to the public. Thanks for asking!

Good luck with your project.

Very Respectfully,

Justin Sta. Ana

	Ph:	(562)278-1545		
Test Automation	Email:	justin@corelis.com		
Engineer	Web:	www.corelis.com		
	Click To	See Virtual card		

Corelis, Inc.

Ri g ht 13100 Alondra Boulevard, Suite 102 Cerritos, CA, USA 90703-2146

I2C Image					-			
Michal Pukala 911electronic <admin@911electronic.com></admin@911electronic.com>				← Reply	Keply All	\rightarrow Forward	ij	
To Juan Rest	To Juan Restrepo Diaz Mon 4/24/2023 9:						:47 AM	
Start your reply all with:	Great, thank you so much!	Okay, thank you! Thank you	i so mu	ich! (i) Fee	dback			
Hi,								ĺ
You can use that in you	r references. I'm happy to se	e that my articles are useful.						
Best regards, Michal								
On 04/24/2023	4:27 AM CEST Juan Restrep	o Diaz <juanfeliperd@knights.< td=""><td>ucf.edu</td><td><u>u</u>> wrote:</td><td></td><td></td><td></td><td></td></juanfeliperd@knights.<>	ucf.edu	<u>u</u> > wrote:				
Hi!								_
My name is Juan Restrepo from the University of Central Florida, and I am a senior in electrical engineering. I am working on a project for my Senior Design class along with teammates and doing our research we would like to ask for your permission to use the figure listed depicting the I2C connections functionality drawing. I would like to emphasize that your site, 911electronic, will be properly referenced and of great help! If there is anything else you need, please let me know.								
Thank you,								
Juan								
Michal Pukala Admin of 911electronic	.com							
mp@911electronic.com	1							