



Gas Chromatography

Matthew McPartlan
Conor Green

ELEC 402: Senior Project
Dr. Asghari

Midterm Presentation

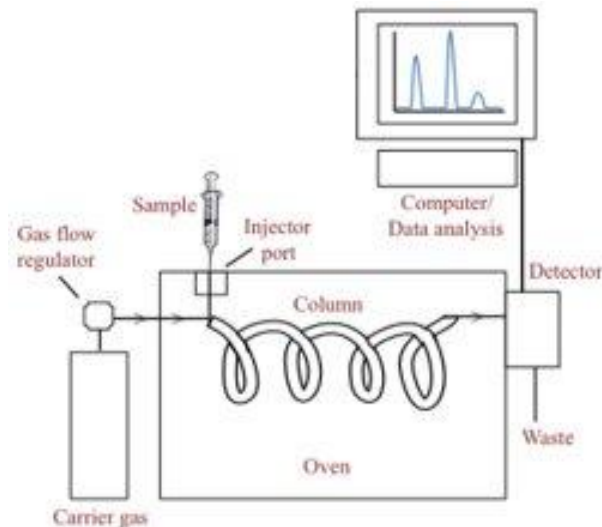
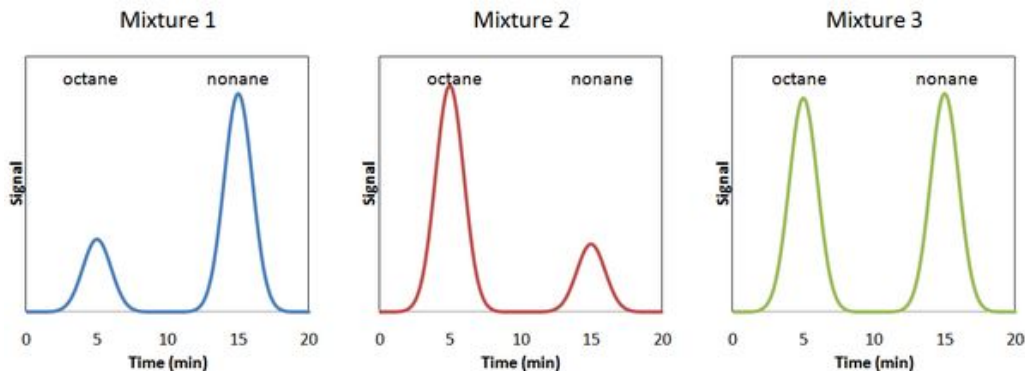


- Background Review
 - Gas chromatography and detector
- Fall Semester
 - Update on detector and carrier gasses
 - Previous prototype
- Spring Semester
 - Colorimetric array
 - Current prototype
 - GUI, ADC, and software
- Future



Reminder: Gas Chromatography is a Separatory Technique

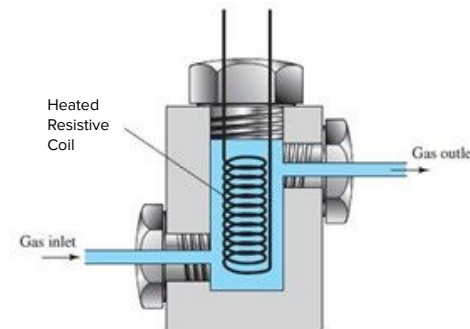
- Allows qualitative and quantitative analysis of solutions with volatile components





Reminder: Detector Operating Principle

- Diode thermal conductivity detector
 - Does not require an inert carrier gas
 - Rugged enough for classroom use
 - Cheap and simple to replace
 - Poor sensitivity
 - Increased sample volume can mitigate this somewhat
- Note:
 - Dried air ($32\text{mW}/(\text{m}^*\text{K})$ @ 125°C)



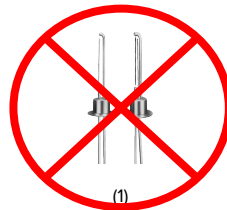
Compound	25°C	125°C	225°C
Acetone	11.5	20.2	30.6
Methane	34.2	49.1	66.5
Methanol	-	26.2	38.6
Ethanol	14.4	25.8	38.4
Hexane	-	23.4	35.4

Thermal Conductivity of Common Analytes
($\text{mW}/(\text{m}^*\text{K})$)

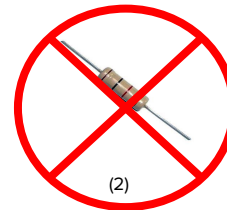


Updated Detector Selections

- ~~Rhenium-tungsten~~
- ~~Carbon-film resistor~~
- 1N4148 Diode



(1)



(2)

Updated Carrier Gas Selections

- Dried air (32 @ 125C)
- ~~Nitrogen (32 @ 125C)~~
- ~~Helium (190 @ 125C)~~



(3)

(1) <https://www.bucksci.com/products/tcd-filament-tungsten-rhenium-includes-seal>

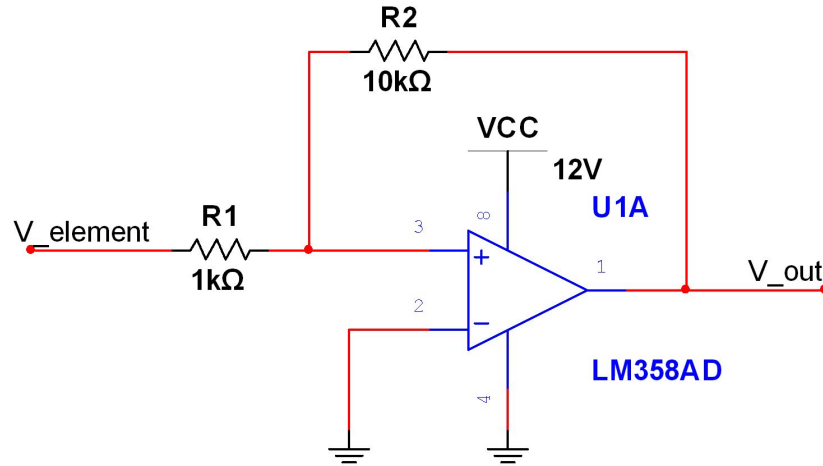
(2) <https://www.westfloridacomponents.com/G530APF08/2W+15K+ohm+Carbon+Film+Resistor+Paccom+RD200T.html>

(3) <https://www.digikey.com/product-detail/en/on-semiconductor/1N4148TR/1N4148FSCT-ND/9356376>

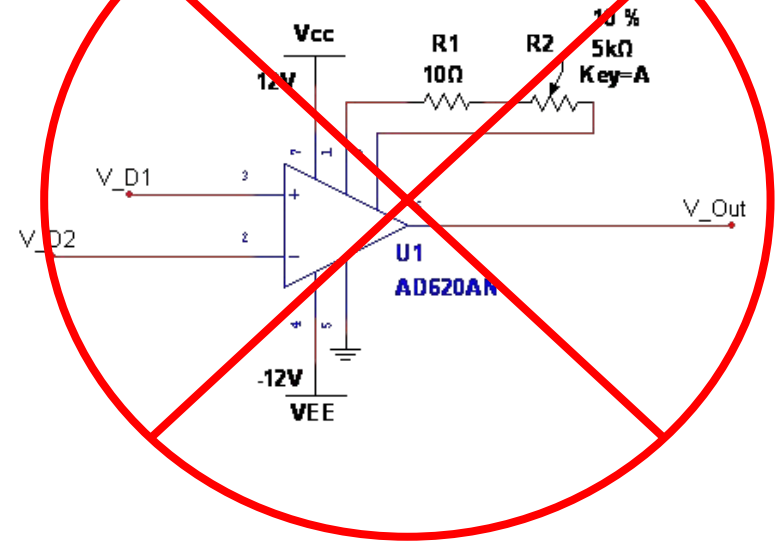


Updated Configuration Selection

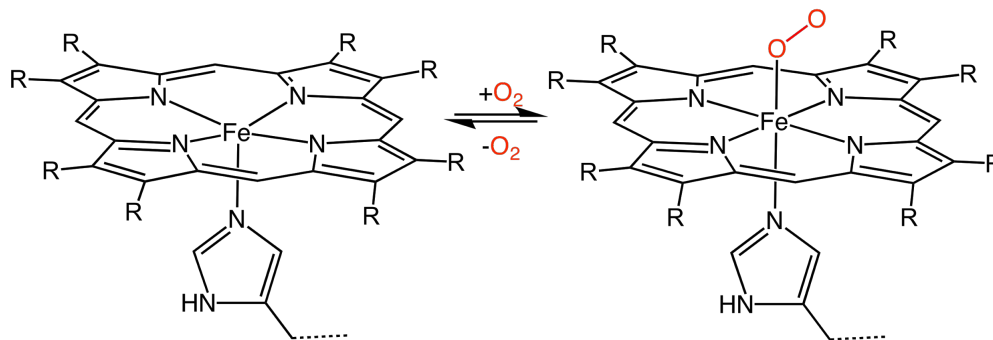
Single-ended



Differential



Reminder: Colorimetric Array Detector

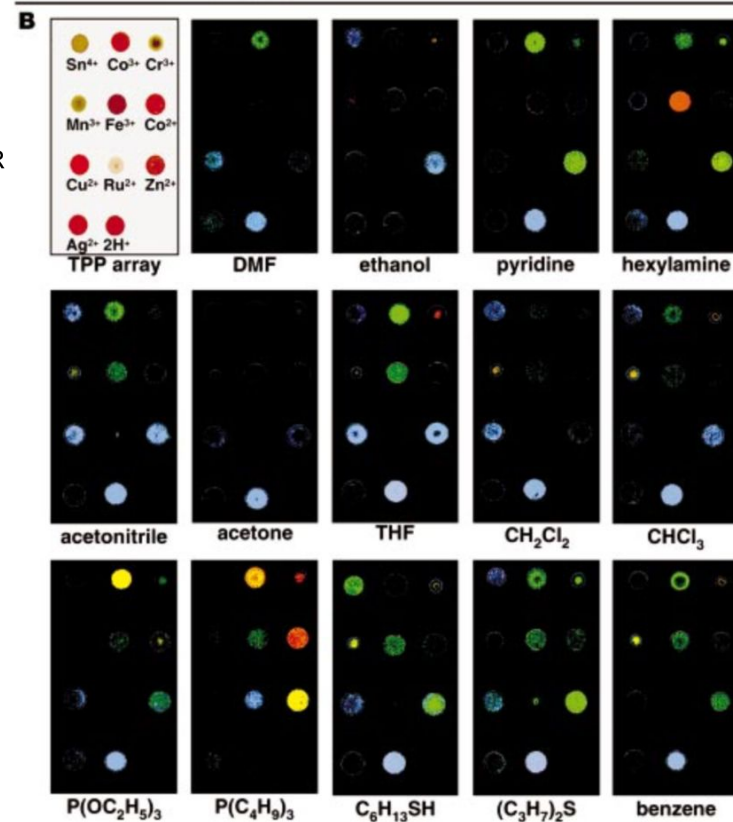


Deoxyhemoglobin

- Dark red
- Fe^{2+} oxidation state

Oxyhemoglobin

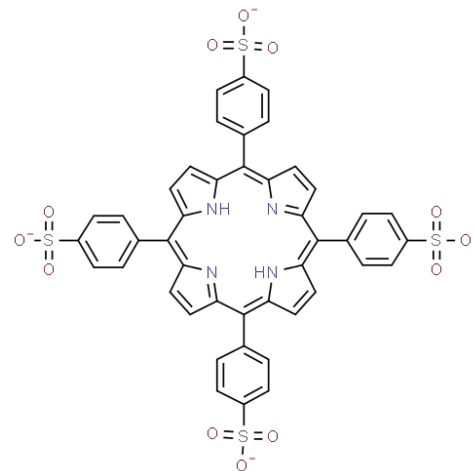
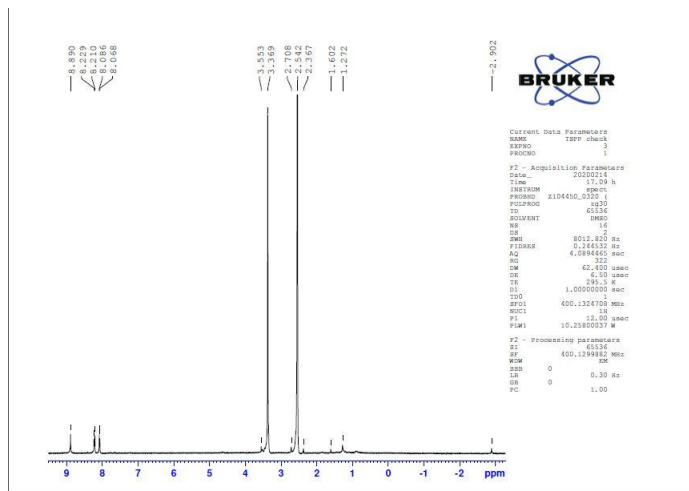
- Bright red
- Fe^{3+} oxidation state
- Oxygen ligand



Progress: Colorimetric Array Detector



- **Innovation:** Sulfonate the metalloporphyrin compounds so they can be dissolved in water.
 - Avoids chloroform, dimethyl sulphoxide (DMSO), and dichloromethane (DCM)



5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin
(Source: ChemSpider)

Testing the Colorimetric Array Detector

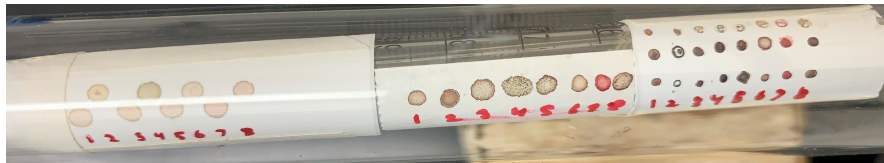


Figure 1: TSPP(Co^{2+}) initial

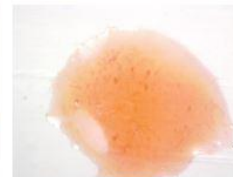


Figure 2: TSPP(Co^{2+}) w/
acetonitrile



Figure 3: TSPP(Co^{2+}) change



Figure 4: TSPP(Fe^{3+}) initial



Figure 5: TSPP(Fe^{3+}) w/
acetonitrile



Figure 6: TSPP(Fe^{3+}) change



Figure 7: TSPP(Ni^{2+}) initial



Figure 8: TSPP(Ni^{2+}) w/
acetonitrile

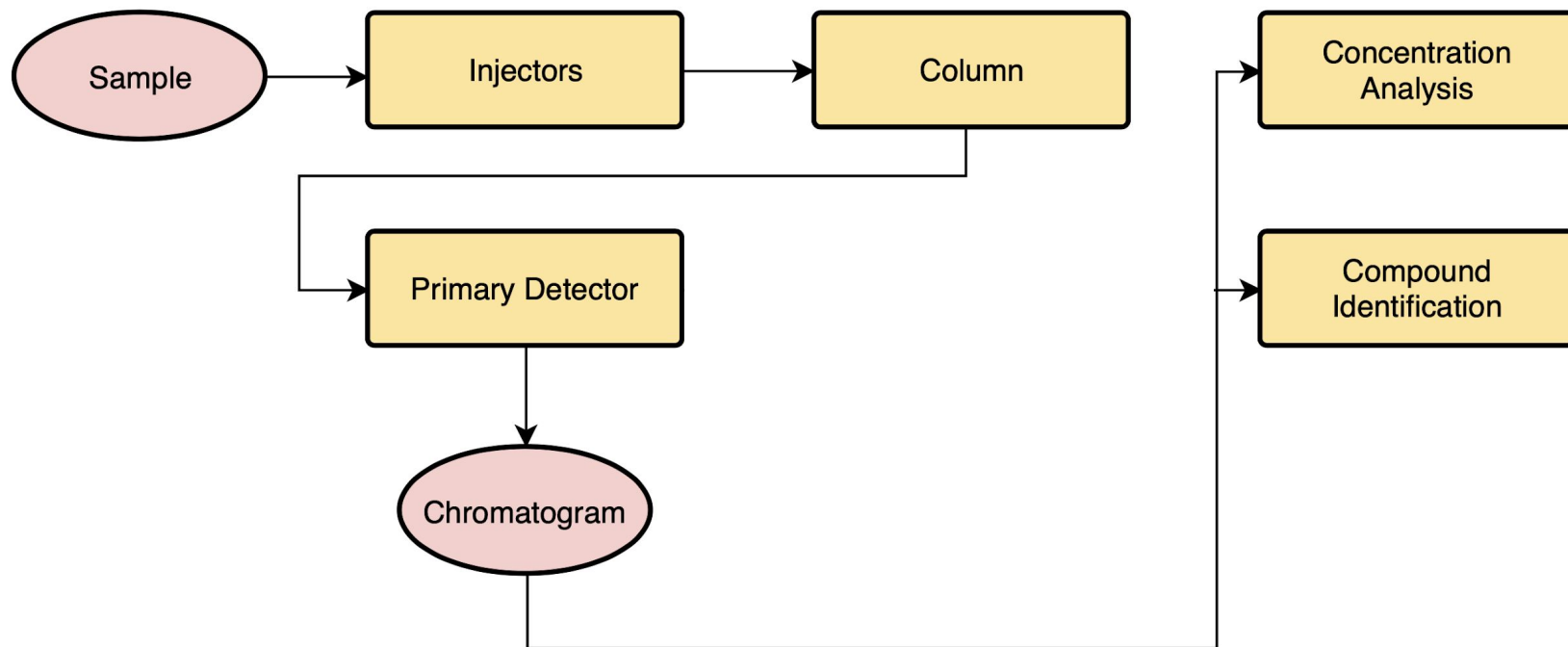


Figure 9: TSPP(Ni^{2+}) change

Unfortunately, this work can not be continued without lab access.



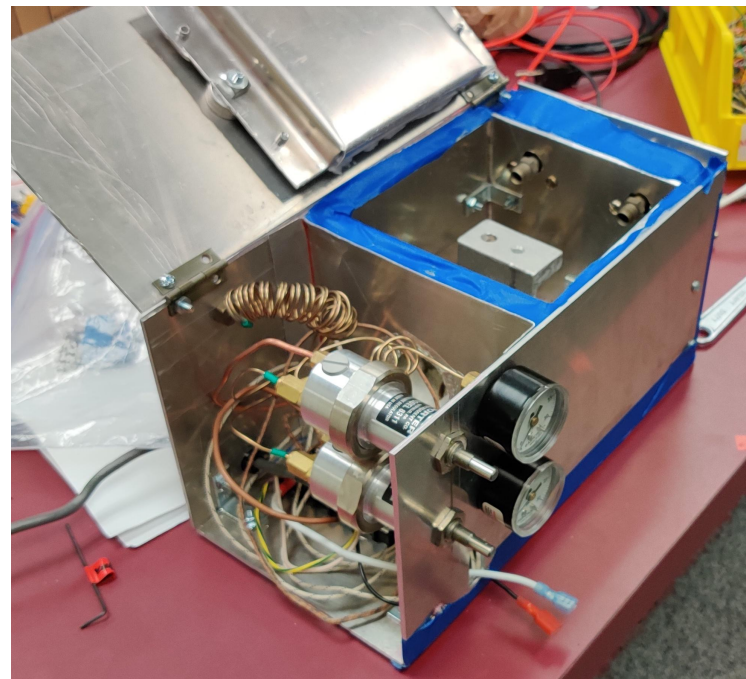
System and Components





Previous Prototype

- Original design and fabrication
- Functional
 - Heating
 - Insulation
 - Gas flow control
 - Configurable detector



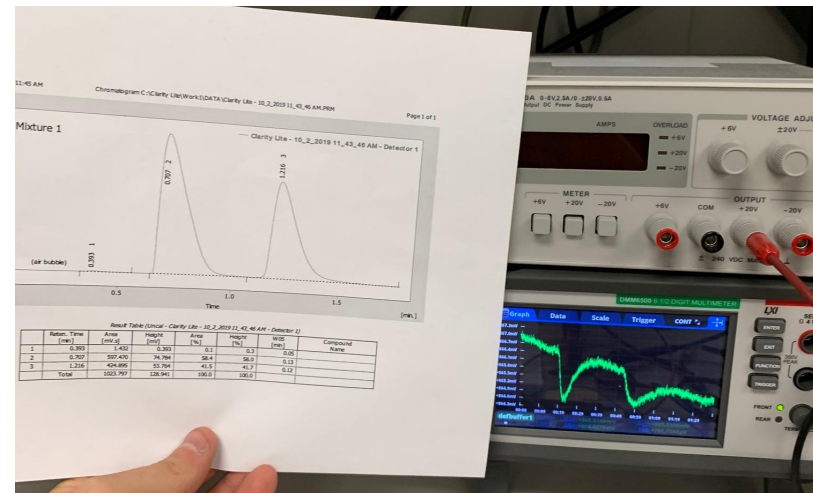


Previous Chromatograms

Single Diode and Nitrogen



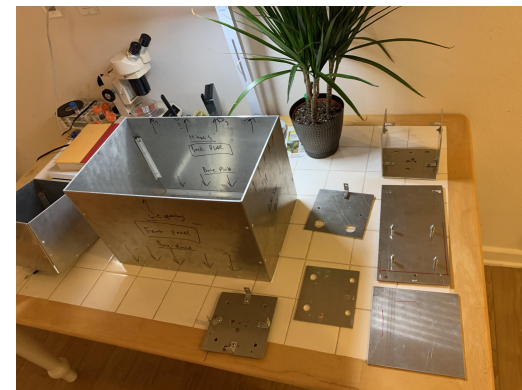
Single Diode and Helium





New Prototype (In Progress)

- Much larger than first prototype
 - Supports a larger $\frac{1}{4}$ " silica separatory column
- Better oven temperature gradient
 - Will not overheat parts of the column
- Not yet complete, but work will continue

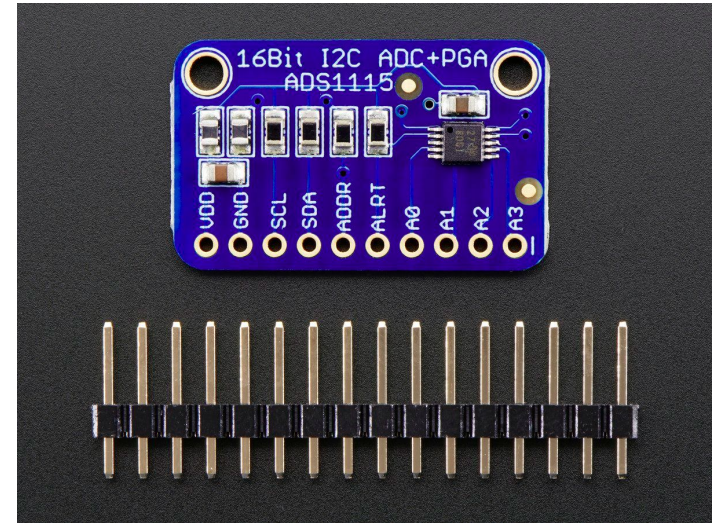


Analog to Digital Conversion



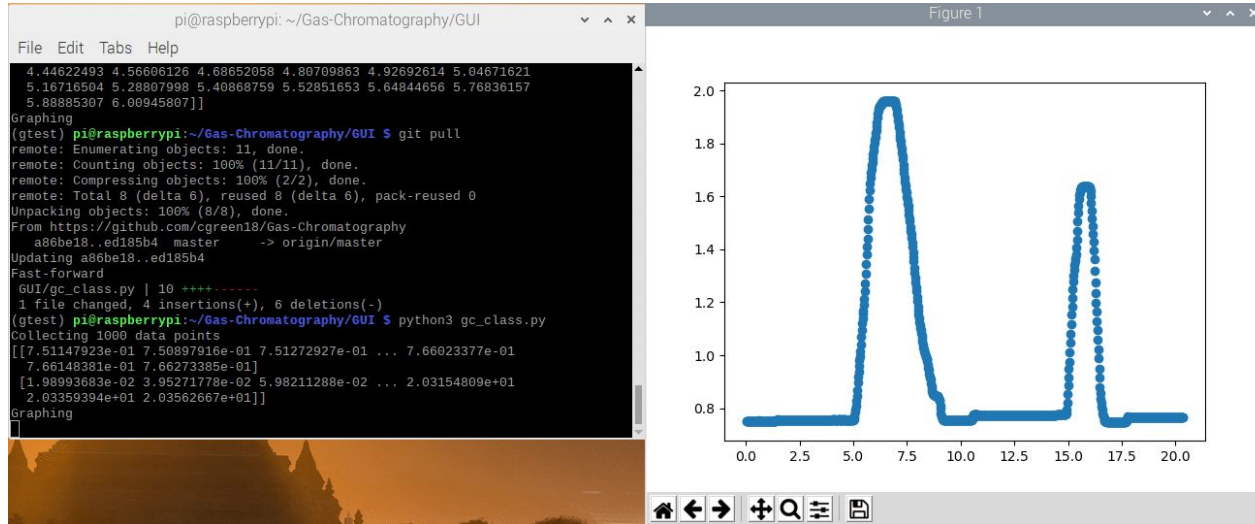
ADS1115

- 16-bit precision analog voltage measurement
- I²C Communication
- Raspberry Pi Library



<https://cdn-shop.adafruit.com/1200x900/1085-03.jpg>

User Interface and GUI



- Python class inherits wxPython and maintains internal variables of previous runs
- Can perform operations on data (e.g. average)

Full Stack



Fresh Raspberry Pi

Install and
Configure scripts

Reboot and Autorun
on startup

```
echo "Install script to set up a new Raspberry Pi to collect gc data and run the gc suite upon startup."
echo "Install instructions given at https://github.com/cgreen18/Gas-Chromatography/tree/master/Installation"
echo "Tested on Raspberry Pi Model 3B+ w/ Raspbian 10 Buster"
echo "20 February 2020 Conor Green"
```

```
jam@jamoney: ~/Documents/Capstone/Gas-Chromatography/Installation
File Edit View Search Terminal Help
./install.sh: line 53: `echo "Building wxPython. Will take a long time (~1-2 hrs)""
jam@jamoney:~/Documents/Capstone/Gas-Chromatography/Installation$ sudo nano ./install.sh
jam@jamoney:~/Documents/Capstone/Gas-Chromatography/Installation$ sudo ./install.sh
Install script to set up a new Raspberry Pi to collect gc data and run the gc suite upon startup.
Install instructions given at https://github.com/cgreen18/Gas-Chromatography/tree/master/Installation
Tested on Raspberry Pi Model 3B+ w/ Raspbian 10 Buster
20 February 2020 Conor Green

Updating repos
Hit:1 https://download.virtualbox.org/virtualbox/debian bionic InRelease
Hit:2 https://packages.microsoft.com/repos/vscode stable InRelease
Hit:4 http://security.ubuntu.com/ubuntu bionic-security InRelease
Hit:5 http://ppa.launchpad.net/gezakovacs/ppa/ubuntu bionic InRelease
Hit:6 http://us.archive.ubuntu.com/ubuntu bionic InRelease
Hit:7 http://us.archive.ubuntu.com/ubuntu bionic-updates InRelease
Hit:8 http://archive.canonical.com/ubuntu bionic InRelease
Hit:9 http://us.archive.ubuntu.com/ubuntu bionic-backports InRelease
Hit:3 https://packagecloud.io/AtomEditor/atom/any any InRelease
Hit:10 http://us.archive.ubuntu.com/ubuntu bionic-proposed InRelease
Ign:11 http://ppa.launchpad.net/wxformbuilder/release/ubuntu bionic InRelease
Ign:12 http://ppa.launchpad.net/wxformbuilder/wxwidgets/ubuntu bionic InRelease
Err:13 http://ppa.launchpad.net/wxformbuilder/release/ubuntu bionic Release
404 Not Found [IP: 91.189.95.83 80]
Err:14 http://ppa.launchpad.net/wxformbuilder/wxwidgets/ubuntu bionic Release
pip install -U pip
```

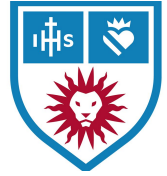
```
# Install dependencies
```

```
apt-get update
```

```
pip install -U six wheel setuptools
```

```
apt-get install build-essential tk-dev libncurses5-dev libncursesw5-dev libreadline6-dev libdb5.3-dev libgdbm-dev libsqlite3-dev
apt-get install dpkg-dev build-essential libjpeg-dev libtiff-dev libssl1.2-dev libgstreamer-plugins-base0.10-dev libnotify-dev t
```


User Interface and GUI



		*Scores are out of 5																	
Design Criteria	Weight (%)	C		Visual Basic		Java		Swing		Python		TkInter		Pygame		PyGtk		wxPython	
		C#				AWT				Qt									
Cross-platform compatability	40	1	0.4	1	0.4	3	1.2	3	1.2	5	2	5	2	1	0.4	4	1.6	5	2
Compilable	5	5	0.25	5	0.25	5	0.25	5	0.25	2	0.1	2	0.1	1	0.05	5	0.25	3	0.15
Speed	20	5	1	4	0.8	1	0.2	1	0.2	2	0.4	2	0.4	2	0.4	3	0.6	3	0.6
Codability	10	3	0.3	3	0.3	2	0.2	2	0.2	4	0.4	4	0.4	5	0.5	3	0.3	3	0.3
Range of abilities	25	5	1.25	5	1.25	4	1	4	1	4	1	4	1	3	0.75	5	1.25	5	1.25
	Total:		3.2		3		2.85		2.85		3.9		3.9		2.1		4		4.3

- wxPython
- Raspberry Pi
- Interface with Arduino Pro Micro via GPIO for analog voltage measurements



Development Plan

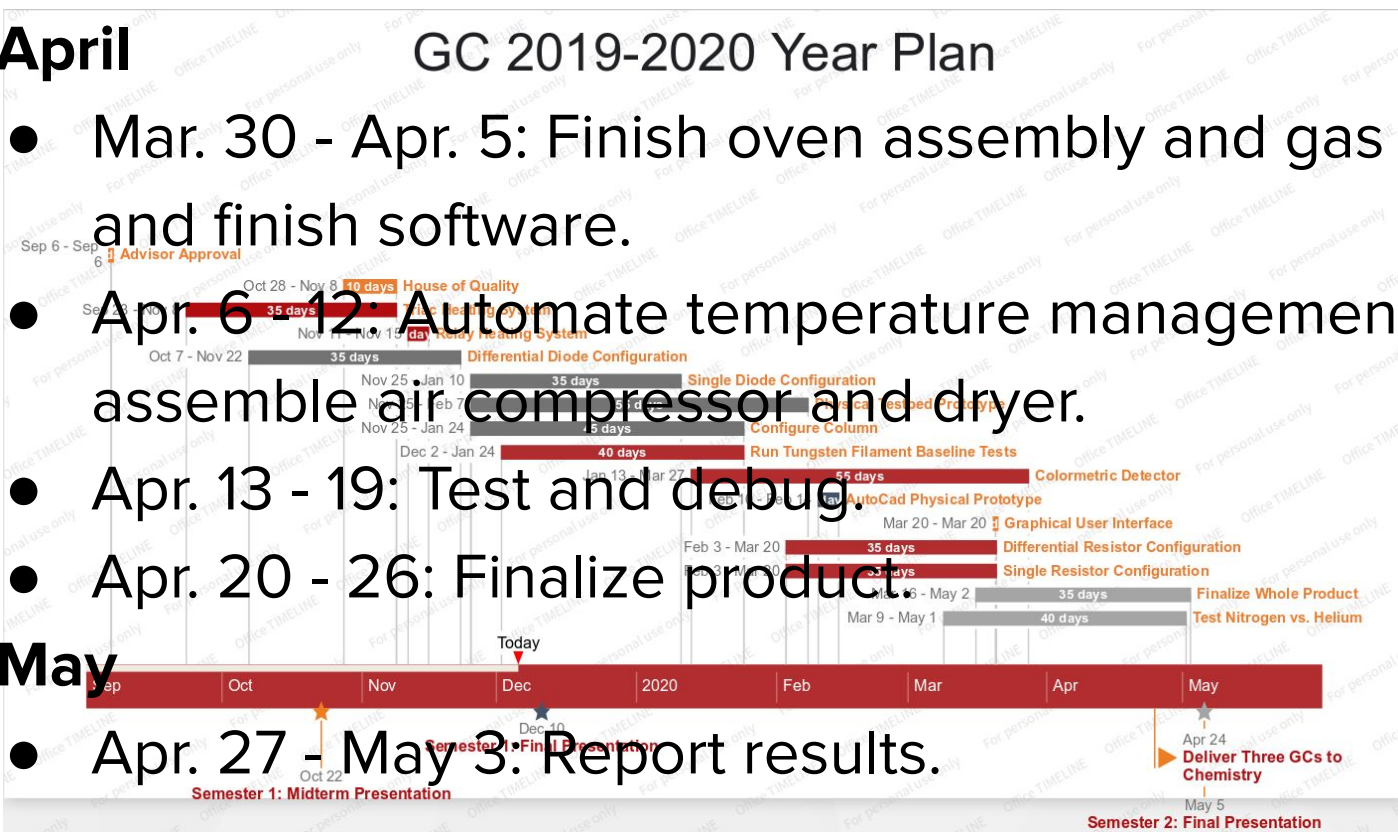
April

GC 2019-2020 Year Plan

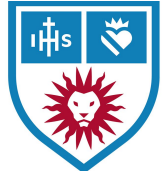
- Mar. 30 - Apr. 5: Finish oven assembly and gas routing and finish software.
- Apr. 6 - 12: Automate temperature management and assemble air compressor and dryer.
- Apr. 13 - 19: Test and debug
- Apr. 20 - 26: Finalize product

May

- Apr. 27 - May 3: Report results.



Looking Forward



Date	Objective
Mar. 30 - Apr. 5	Finish oven assembly and gas routing and finish software
Apr. 6 - 12	Automate temperature management and assemble air compressor and dryer
Apr. 13 - 19	Test and debug
Apr. 20 - 26	Finalize product
Apr. 27 - May 3	Report results



References

K. Rakow, N. & Suslick. A colorimetric sensor array for odour visualization. *Nature*, 406:710–713, August 2000.

M. Jones. A simple-to-build thermal-conductivity gc detector. *Journal of Chemical Education*, 71:995–996, November 1994.

Objectives



- **Simple:** Student can operate
- **Accurate:** Detects impurities $\geq 5\%$ of substance
- **Carrier gas:** Air > nitrogen > helium
- **Safe**
- **Durable and serviceable:** ≥ 2 weeks uptime / service
- **Economic:** $\leq \$500$ /instrument
- **Documentation**