UV-Visible Light Absorbance Analysis of Water Quality and PACE OCI Hyperspectral Data Analysis and Classification

Annika Means, Oliver Wang
Mentors: Changyong Cao, Xi Shao, Sirish Uprety, Chun-Kai Hsu

Objectives

- Assess water quality using UV-Vis Absorbance Spectroscopy
- Analyze absorbance data to determine presence of constituents:
  - CDOM, phycocyanin, phycoerythrin, salinity, temperature, turbidity, and hazardous water contaminants
- Explore how water quality differs across regions
- PACE OCI data analysis and classification

Motivation

- Water contaminants are detrimental to human and ecosystem health
- Contaminated water may appear clean, and its consumption can lead to waterborne disease outbreaks and illness
- Cost-effective methods for water quality detection

Absorbance:
Amount of light absorbed; describes sample composition.

Beer-Lambert Law:

$$A = \varepsilon c l$$

A = absorbance
ε = molar extinction coefficient
c = concentration
l = length of the light path

Methods

- Collected water samples from rain, streams, creeks, taps, ponds, and lakes
- Analyzed absorbance of samples using spectrometer

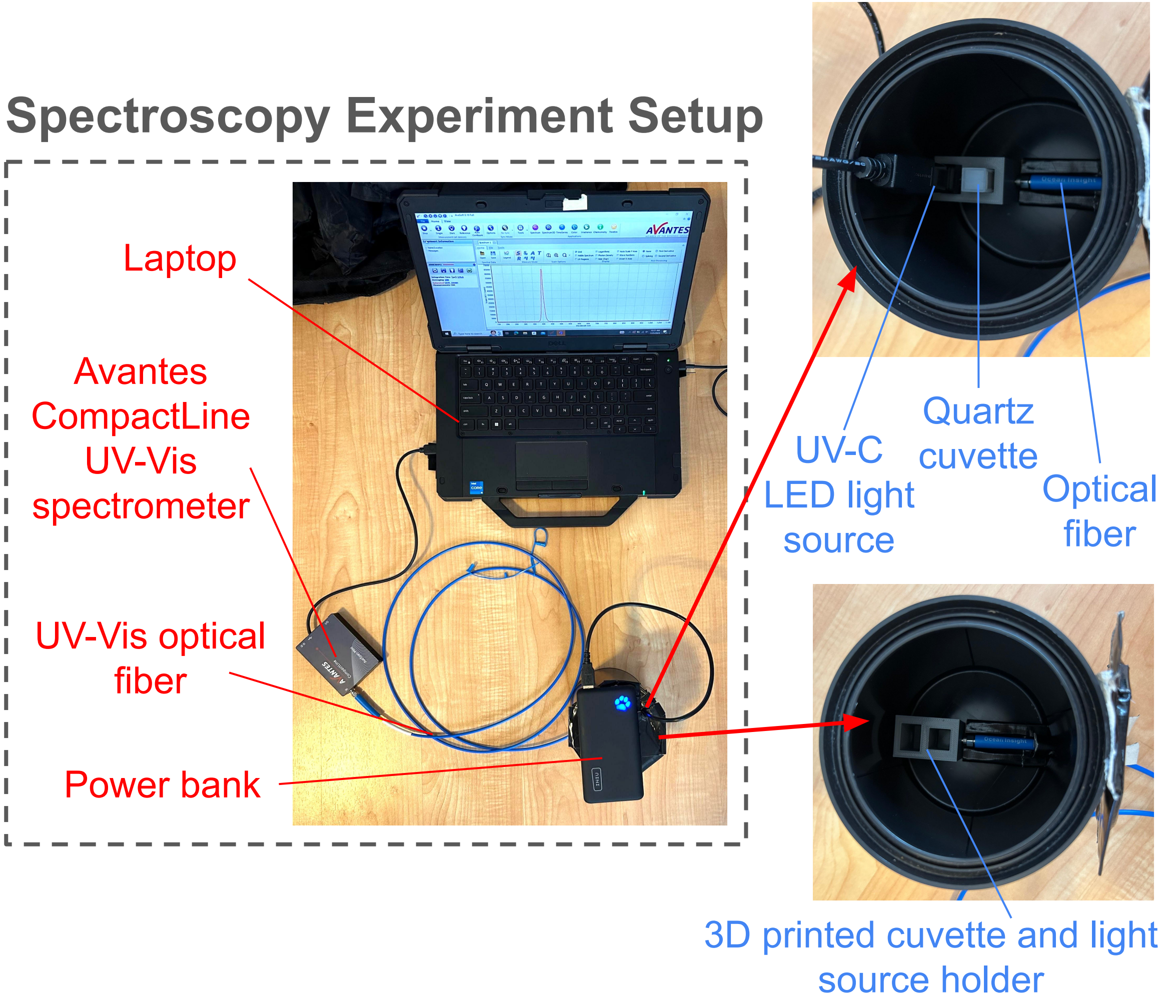
Water Collection

Brookside Gardens

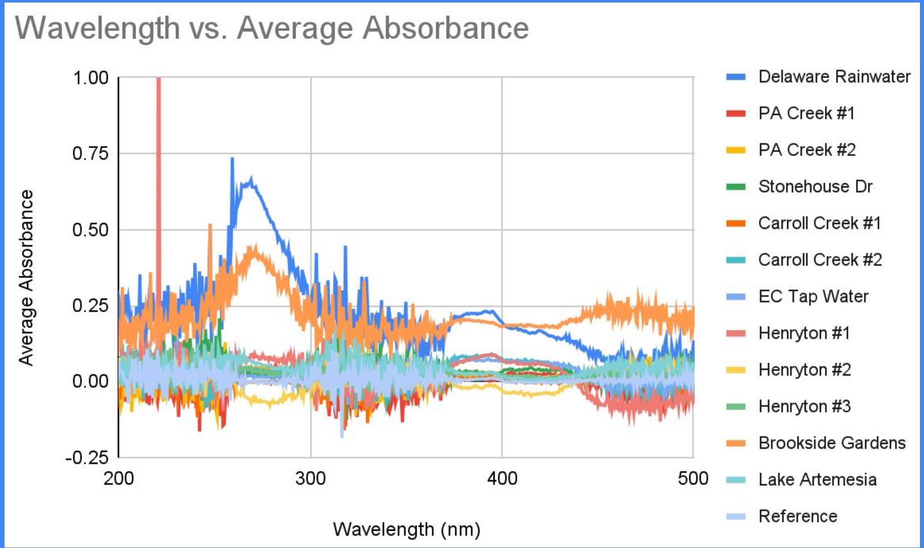
Stonehouse Drive

Spectroscopy Experiment Setup

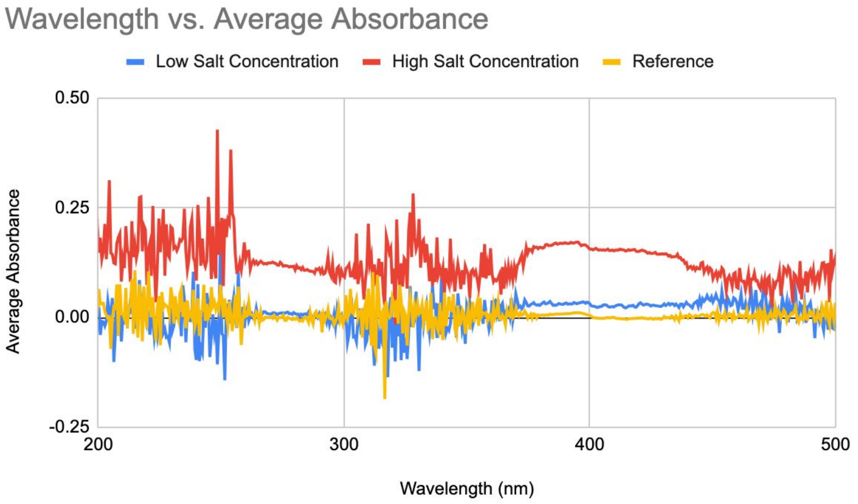
Box Interior:

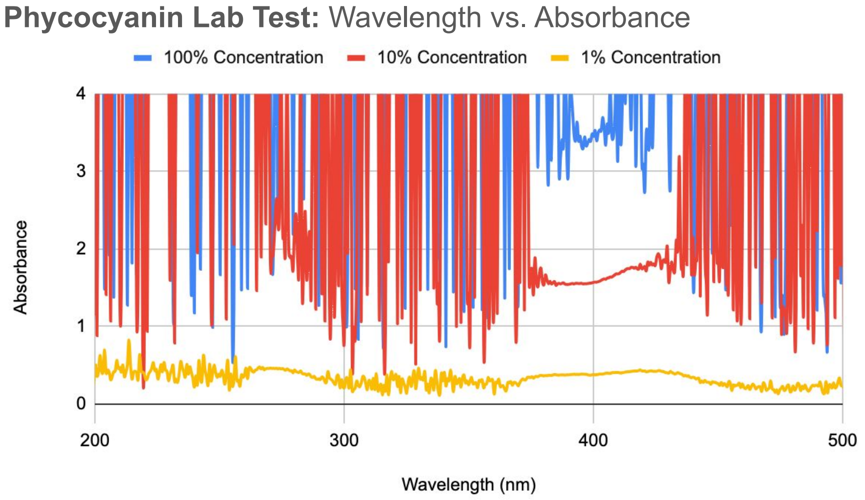


Results



All fieldwork samples from 200 nm to 500 nm





Parameters

Relative concentration of components, based on absorbance at specific wavelengths:

- Very High: ≥ 0.500
- High: 0.150 - 0.499
- Moderately High: 0.100 - 0.150
- Moderate: 0.050 - 0.099
- Moderately Low: 0.025 - 0.049
- Low: 0.000 - 0.024

Wavelengths of Peak Absorbance for Constituents of Interest: from Literature Review

Component	Peak Absorbance Wavelength (nm)	Actual Wavelength Assessed (nm)
CDOM	254	253.9
C-PC	620	619.77
R-PC (533 nm)	533	532.84
R-PC (544 nm)	544	544.19
Allophycocyanin	652	651.75
PE545	545	544.79
B-PE	545	544.79
R-PE	565	565.07
NaCl	197	197.13
NaOH	201	200.8

Component	Peak Absorbance Wavelength (nm)	Actual Wavelength Assessed (nm)
Chlorophyll a (412 nm)	412	412.16
Chlorophyll a (663 nm)	663	662.98
Nitrate	220	219.74
Nitrite	354	354.14
Lead	538.52	538.82
Lead (UV region)	211	211.19
Copper	619.89999	619.77
Copper (UV region)	221	220.96
Arsenic	617	616.8

Sources: (Eijckelhoff & Dekker, 1997; Eurogentec, n.d.; Lace et al., 2019; *Product Data Sheet: C-Phycocyanin*, n.d.; *Refractive Index and Extinction Coefficient of Materials*, n.d.; Shi et al., 2022; Stadnichuk et al., 2020; *SureLight® Allophycocyanin (APC)*, n.d.; *SureLight® B-Phycoerythrin (B-PE)*, n.d.; Tan et al., 2014; Tong et al., 2020; Yeshno et al., 2019; Zagurskaya-Sharaevskaya & Povar, 2015; Zuo & Deng, 1998)

Results Analysis

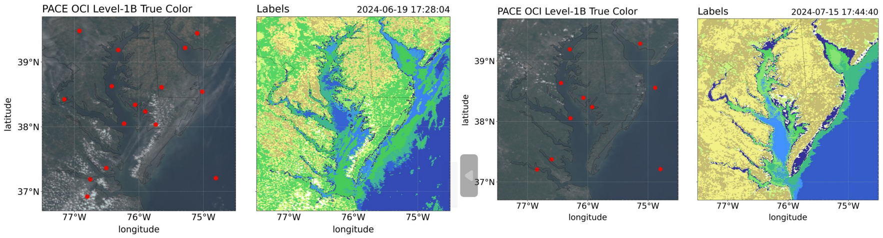
Sample	Appearance	Possibly Very High Concentration	Possibly High Concentration
Delaware Rain	Clear	N/A	**Nitrate, CDOM, copper, C-phycocyanin, allophycocyanin, lead (UV), chlorophyll a (412 nm)**
Stonehouse Stream	Clear	**Chlorophyll a (663 nm)**	N/A
Henryton Stream (Cuvette #1)	Mostly clear, some small brown particles	**Nitrate, chlorophyll a (663 nm)**	**Copper (UV)**
Brookside Pond	Yellow green, visible particles (grass, dirt)	N/A	**Nitrate, CDOM, nitrite, chlorophyll a (412 nm), phycoerythrin 545, B-phycoerythrin, allophycocyanin, lead (UV)**

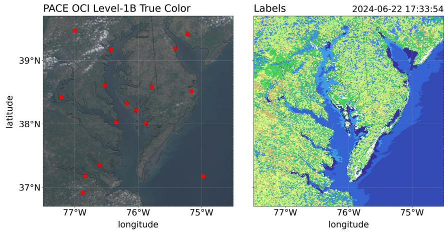
Conclusions

- Delaware Rainwater and Brookside Gardens Pond were the most contaminated samples
- UV-Vis absorbance spectroscopy is a cost-effective method for assessing general water quality
- Appearance does not always correspond to water quality
- Absorbance cannot explain all aspects of a sample
  - Undissolved particles
  - Detect constituents that are not actually present
  - Noise
- Absorbance should be used in conjunction with reflectance, transmittance, and other measurement techniques for more accurate water quality analysis

PACE OCI Hyperspectral Imaging and classification over the Chesapeake Bay area

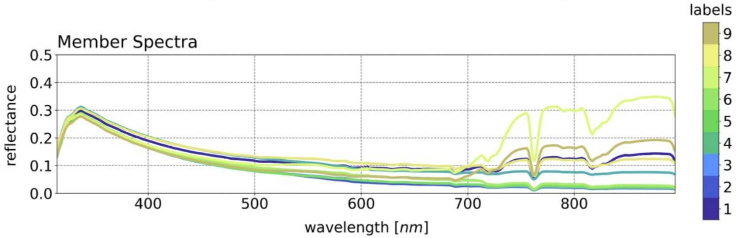
Classified Maps:





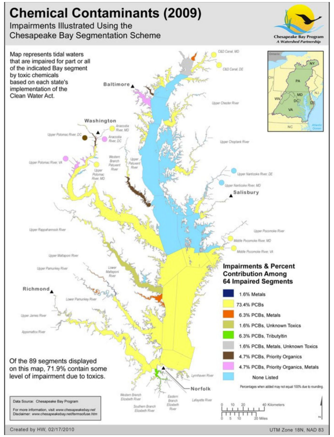
Procedure:
Create true-color plots
Extract spectral signatures from manually selected locations
Run the spectral signatures through the SAM (Spectral Angle Mapper) Classification method to generate classified maps from hyperspectral data

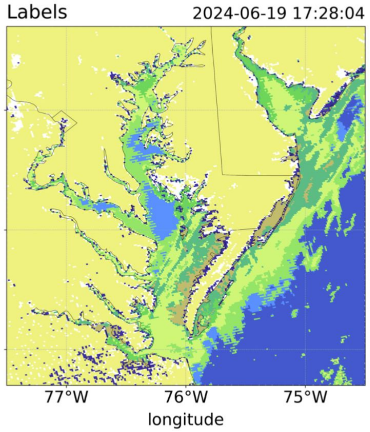
Spectra extracted from selected locations:



Comparison with Other Classifications of Chesapeake Bay Area

Water Classification Map:





Land Classification Map: