

Internet of Things Course

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SAPIENZA
UNIVERSITÀ DI ROMA

Group Project Fish Farming Water Monitoring

Course of Internet of Things

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Fish Farming Water Monitoring

Using Spectrophotometer for Underwater Quality
Analysis



Aquaculture 4.0

- Farmers traditionally performs periodic on site measurements/inspections of water quality
- Traditionally Technical staff are composed by veterinaries, biologists, chemists using hand held instruments
- Aquaculture 4.0 means unmanned 24/24 hours aquaculture monitoring
- Real time data and complete historical data base
- Triggering of alarms when hazardous situations and immediate correction



Water Quality Parameters

- Fitoplankton and Zooplankton
- Oxigene percentage (optimum 80%-120%)
- Ph(6.5 – 9), Salinity (5g/L – 40g/L), Alkalinity(50-250mg/L)
- Waste : Droppings and uneaten feeds
- Oil
- Heavy metals (mercury), Dioxins, Polychlorinated biphenils, Pesticides
- Nitrogen dioxide, Nitrogen Catabolites, Ammonia (0-0.03)
- Turbidity (suspended solids or plankton) less than 1 NTU not more than 5 NTU
- Temperature (optimum 25° C - 35° C)



Water Color Detection

So we have seen the water quality parameters. Now we are interested that the spectrophotometer Having a qualitatively and quantitatively unknown water sample is able to determine which quality parameters are present and possibly in what percentage. This is why in our case we have oversimplified. That is, we have moved the determination of the quality parameters to a single quality parameter, taking the color of the water as an example. So if our spectrophotometer will be able to determine the color of an unknown water sample and possibly the quantity of color or the color density of that sample, we would have solved our problem. In other words, we could therefore solve the problem of determining the presence in a sample of water of the presence of petrol for example and in what quantity. Because the process will be the same.



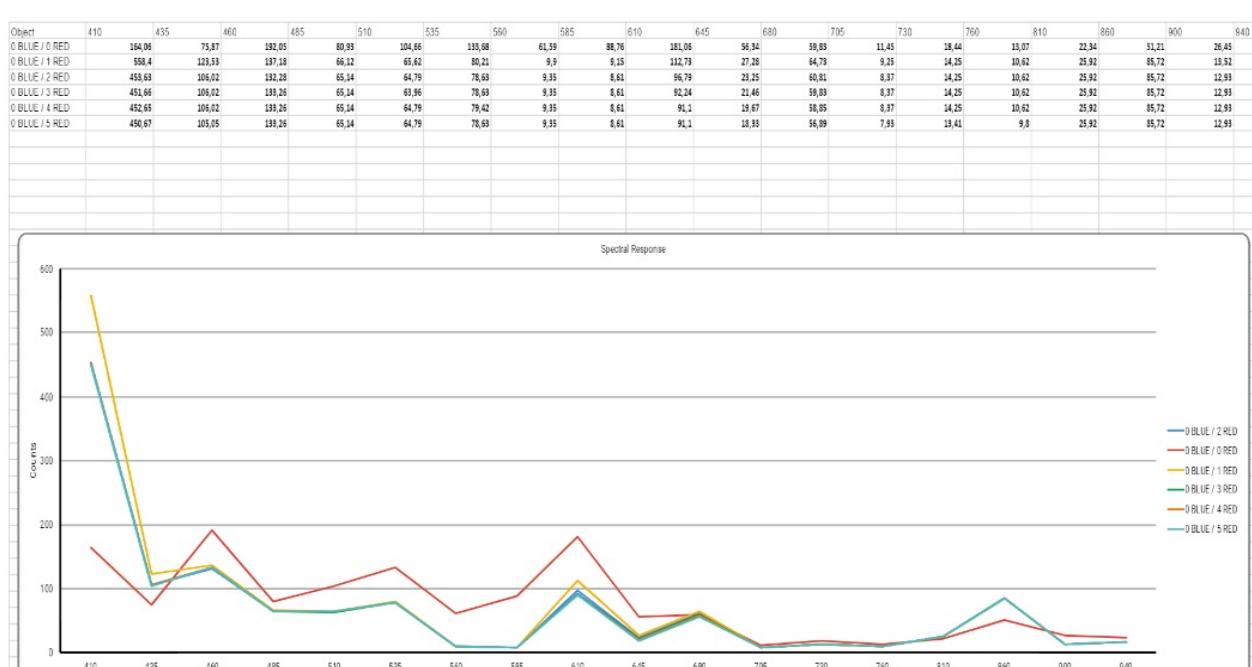
Set up of the in-container Lab Experiment



Two types of experiments were performed. A first experiment by adding to each tank containing 2 liters of water a gradually increasing quantity of dye powder. he tried first with blue, then with red, then with a mixture of blue and red. Finally a second experiment was done. By measuring the different light radiations from 20 different colors.



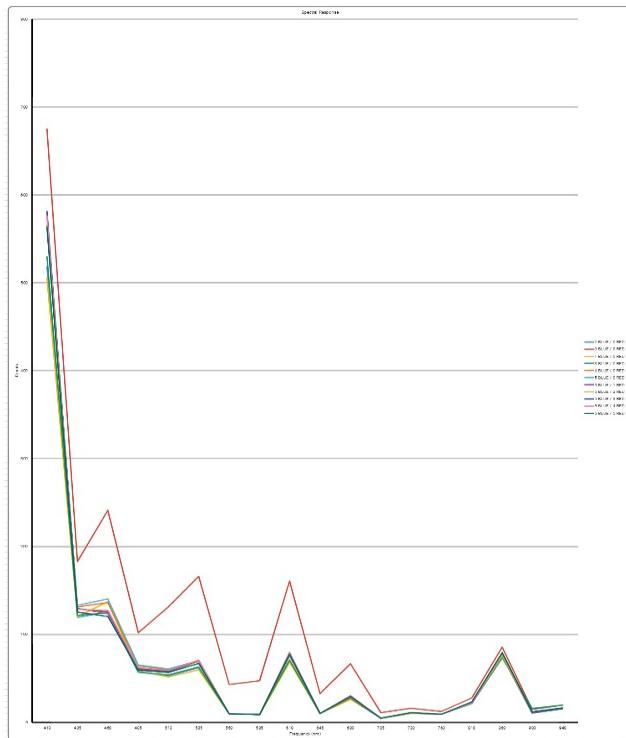
Result of First in-vitro Lab Experiment



from this first graph obtained by adding increasing red values, we infer that the frequencies (410 nm and) 860 nm have a positive linear correlation between the measured intensity and the percentage of red in the aqueous solution. Therefore are the optimal frequencies to detect the concentration of red color in the aqueous solution



Result of First in-vitro Lab Experiment

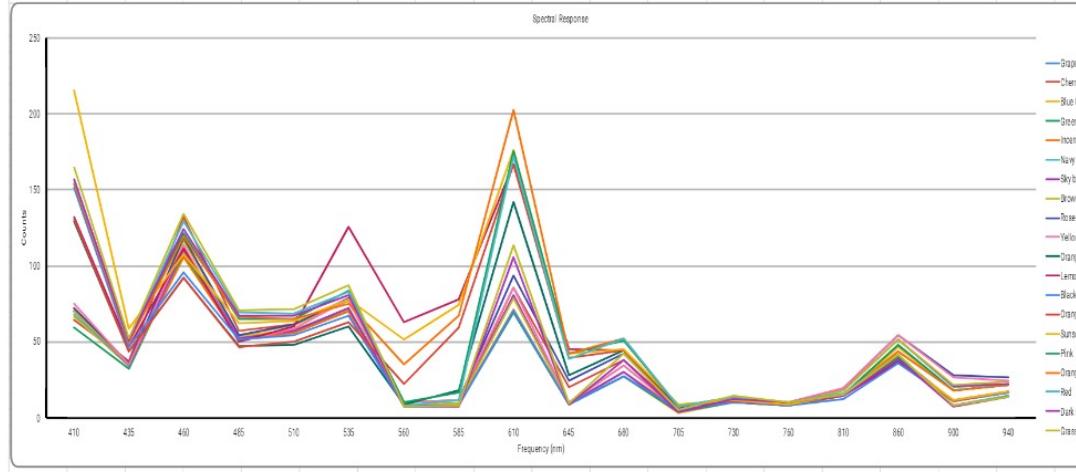


We can determine some wavelength nanometer in the graphic that indicate that by increasing the color concentration leads to an increase in the absorption of light at these wavelength, and this causes a decrease in the intensity of light measured by the spectrophotometer detector



Result of Second in-vitro Lab Experiment

Object	410	435	460	485	510	535	560	585	610	645	680	705	730	760	810	860	900	940
Cherry Red	64.24	36.96	132.28	57.24	61.47	77.06	7.7	8.61	85.4	20.12	38.25	5.72	10.06	8.17	14.3	43.42	17.84	21.4
Blue Green	66.22	34.04	118.56	53.29	58.14	71.56	7.15	8.61	71.74	8.94	27.46	3.08	10.06	8.17	14.3	46.76	17.84	21.4
Grape Purple	70.17	35.02	111.7	53.29	57.31	71.56	7.7	8.61	69.46	8.94	27.46	4.4	10.66	8.17	15.19	47.87	18.22	21.4
Green	59.8	32.1	107.78	52.31	56.48	69.88	7.7	8.61	69.46	8.94	27.46	3.52	10.66	8.17	15.19	47.87	18.22	21.4
Incense Purple	71.16	34.04	105.82	51.92	55.65	69.88	7.7	8.61	70.6	8.94	90.4	4.84	10.9	8.17	15.19	48.42	18.22	21.4
Navy Blue	68.19	34.04	109.74	52.31	57.31	72.34	8.25	9.15	80.85	8.94	30.4	3.52	11.75	8.98	17.87	51.21	18.99	23.38
Sky blue	70.17	34.04	110.72	52.31	57.31	72.34	8.25	9.15	80.85	9.39	80.4	3.52	11.75	8.99	17.87	51.21	20.58	23.38
Brown	70.17	35.02	116.6	54.28	60.64	77.06	8.15	9.15	78.57	9.39	34.59	5.28	11.75	8.99	17.87	51.21	21.75	23.35
Rose	72.15	35.99	118.56	54.28	61.47	78.93	9.9	11.3	95.98	24.99	42.17	8.17	11.57	9.8	19.66	54.55	28.22	23.27
Yellow Green	75.11	35.92	113.66	50.93	58.97	77.35	10.45	11.3	85.4	10.28	34.33	5.23	11.57	9.8	19.66	54.55	28.45	23.32
Orange Red	129.47	43.77	92.11	47.87	48.18	59.76	8.8	18.29	142.84	21.17	44.14	7.49	10.9	8.99	14.3	37.85	18.58	15.54
Lemon Yellow	151.43	46.69	111.7	50.93	59.8	125.81	65.24	70	167.89	44.72	44.14	7.93	10.9	8.99	14.3	36.74	11.76	17.51
Black	151.21	46.69	96.05	51.32	53.99	68.84	7.7	8.07	70.6	8.94	27.46	4.84	10.66	8.17	12.51	35.62	10.58	15.54
Orange	150.46	43.77	92.11	46.39	49.84	61.91	22	59.17	157.39	39.35	44.14	7.93	10.9	8.99	15.19	40.08	11.37	17.51
Sunset Red	215.45	58.36	107.78	62.18	63.96	77.35	51.14	74.24	176.5	41.03	45.12	8.37	11.75	8.99	15.19	38.96	11.76	17.51
Pink	153.19	56.58	121.5	65.14	64.79	83.35	10.45	16.68	175.36	42.48	51	7.49	13.41	8.8	15.19	40.08	8.23	14.59
Orange Yellow	154.18	49.61	119.54	66.12	64.79	74.7	35.2	67.24	102.66	42.03	51.98	7.49	13.41	8.8	16.09	41.19	8.23	14.59
Red	156.15	56.58	129.54	69.09	68.94	82.57	7.7	11.83	171.95	38.9	51.98	7.05	13.41	9.8	16.09	41.19	7.64	14.59
Dark Green	157.14	56.58	124.44	67.11	67.28	85.99	7.15	7.53	105.9	8.94	38.25	8.52	12.57	9.8	14.3	38.96	7.05	14.62
Green Green	165.05	52.53	134.04	72.05	71.43	87.28	7.15	8.07	113.87	9.39	42.17	9.20	14.25	9.8	15.19	41.19	7.54	13.82





Normalization of measurements of the Lab set-up

- The intensity measured by the spectrophotometer detector is dependent on the position of the detector in the container and this can vary from one measurement set-up to another. This is why it is needed a normalization of signal to respect to pure water.
- In order to normalize the value of the signal plotted on the y axis it should be calculated by dividing the value of spectra for pure water by the value of spectra for coloured water.
- $Y = \log ((\text{spectra for pure water}) / (\text{spectra for coloured water}))$



Spectrum wavelenghts

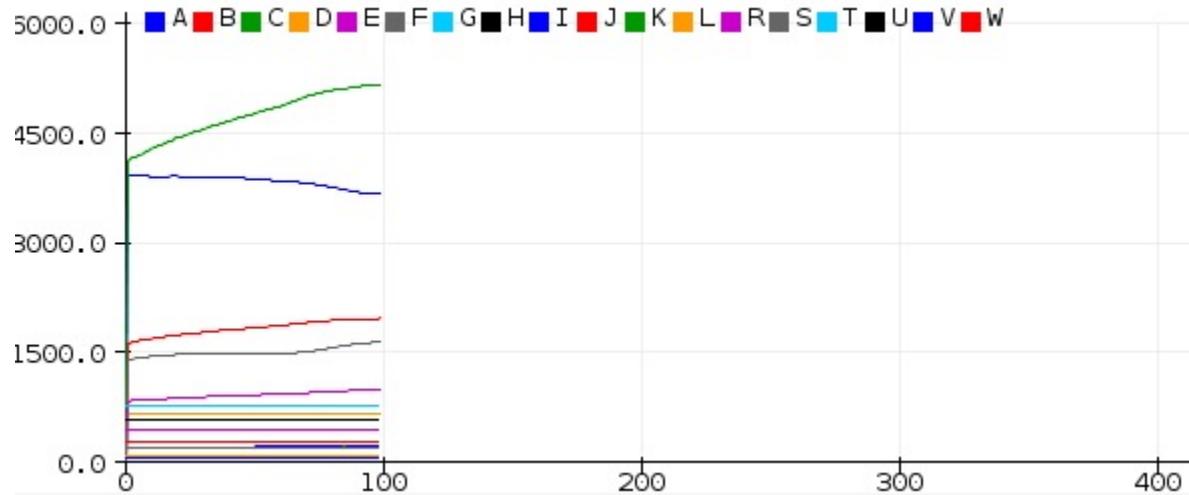
- VIS : visible light sources 400-750 nm

400-430	Violet
430-500	Blue
500-570	Green
570-620	Yellow to Orange
620-670	Bright Red
670-750	Dark Red

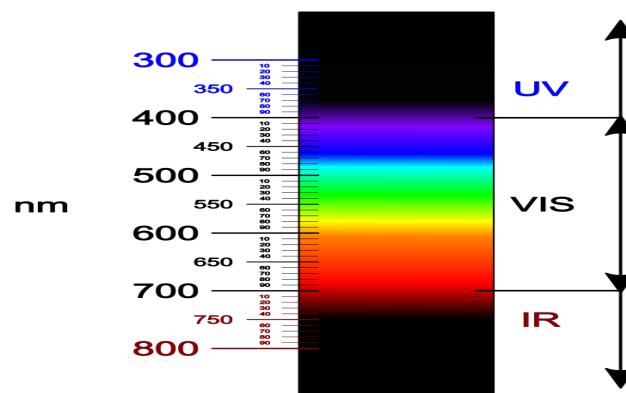
- NIR : near infrared over 750 nm
- UV : ultra violet 340-400 nm
- MIR : mid-infrared over 2500 nm



Trasmittance Measured from water sample in closed space



Device	Channel	Center λ (nm)
AS72653	A	410
AS72653	B	435
AS72653	C	460
AS72653	D	485
AS72653	E	510
AS72653	F	535
AS72652	G	560
AS72652	H	585
AS72651	R	610
AS72652	I	645
AS72651	S	680
AS72652	J	705
AS72651	T	730
AS72651	U	760
AS72651	V	810
AS72651	W	860
AS72652	K	900
AS72652	L	940





Experimental Design and Implementation

- In this experiment I have added a teaspoon of dyes (blue color powder) from 1 to 5 , at each sensor measurement trial
- Therefore we will focus only on optimal wavelengths outcomes , and we will divide the classes in 1 to 5
- The class labels and measured intensity data are then used as input for classification algorithms that result in a classifier for identification of the levels of colours, say low, medium , high



Spectrum wavelengths optimal points

- It can be also noticed that , at some wavelengths, by adding a dyes the intensity of light is higher , while at a different wavelength the same add causes a decrease of intensity. The decrease of intensity signal means that at that wavelength the absorption is higher.
- Therefore the intensity data measured using these wavelengths light sources can be used to achieve a higher sensitivity to colour concentrations.



Colour Prediction Models using Multiple Linear Regression

- The MLR can be used to predict the value of an output based on a linear combination of input variables.
- The input variables are the measured intensity at the optimal wavelengths (1 or more) and denoted as x_1, x_2
- And the output is the color concentration predicted value (y)
- The regression equation will be :

$$y(i) = \theta_0 x_1(i) + \theta_1 x_2(i)$$

Where i represents the i -th data sample



Colour Prediction Models using Multiple Linear Regression

- The objective of the model is to find the best parameters θ that will minimize the mean squared error (MSE).
- It will be necessary to use gradient descent method , as iterative optimization, which gradually updates the model parameters until the prediction error is at a minimum value.
- NOTE: This requires a much more larger data sample!



What is the Beer-Lambert Law ?

The Beer-Lambert law is a linear relationship between the absorbance and the concentration, molar absorption coefficient and optical coefficient of a solution:

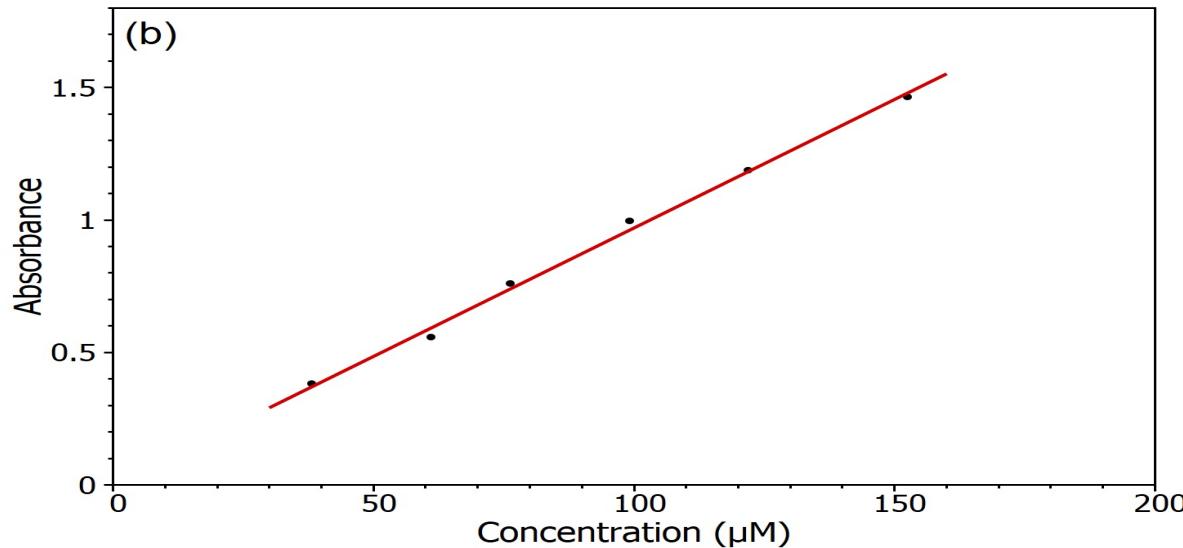
$$A = \varepsilon cl$$

A	Absorbance	
ε	Molar absorption coefficient	$M^{-1}cm^{-1}$
c	Molar concentration	M
l	optical path length	cm



What is the Beer-Lambert Law ?

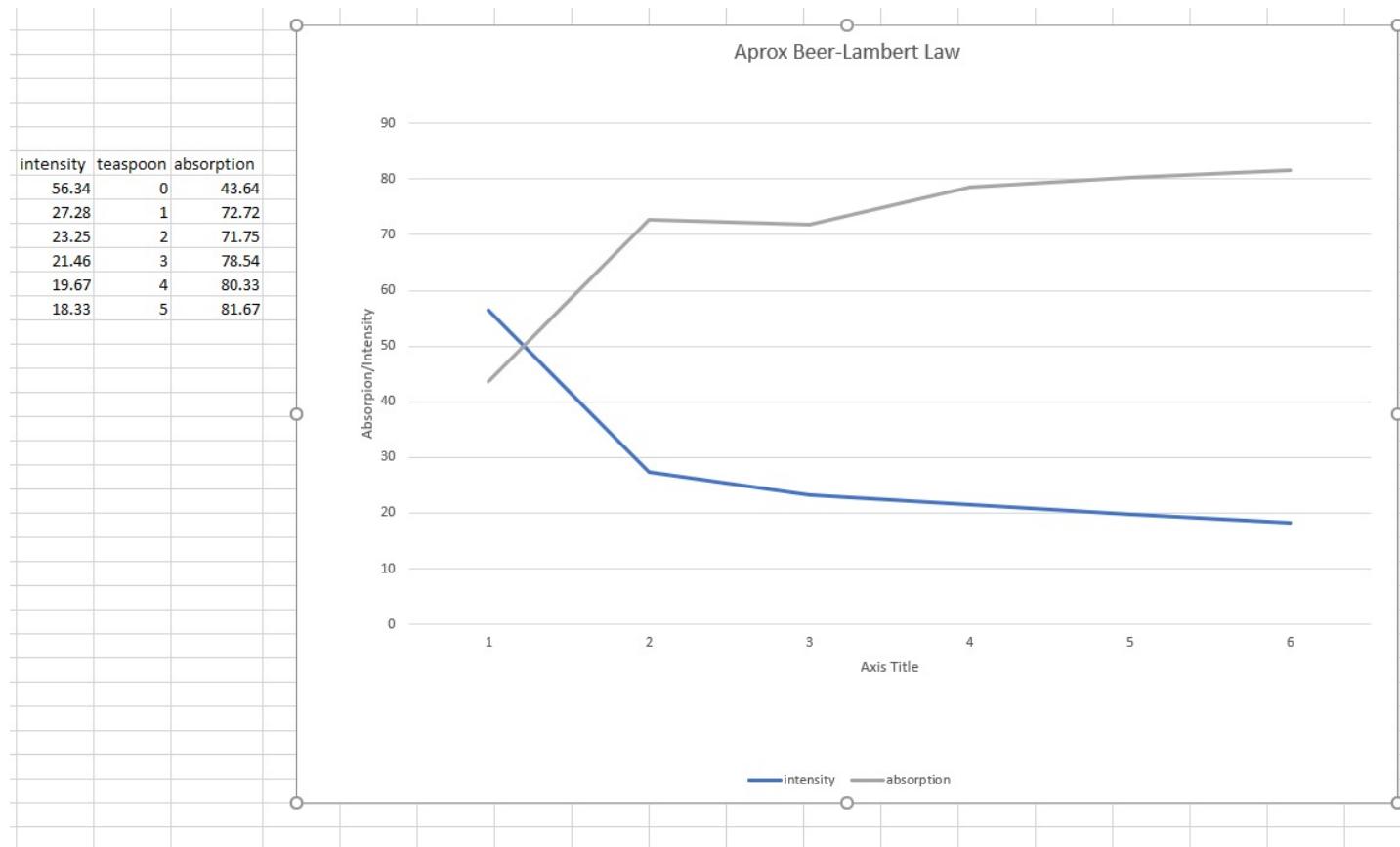
The Beer-Lambert law states that there is a linear relationship between the concentration and the absorbance of the solution, which enables the concentration of a solution to be calculated by measuring its absorbance.



La mole è l'unità di misura della quantità di sostanza.



Approximation of Beer-Lambert Law for Red Colour ?





What is the Beer-Lambert Law ?

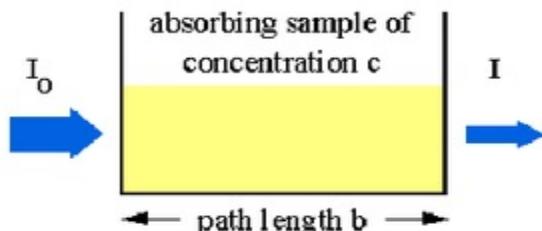
Experimental measurements are usually made in terms of transmittance (T), which is defined as:

$$T = I / I_0$$

where I is the light intensity after it passes through the sample and I_0 is the initial light intensity. The relation between A and T is:

$$A = -\log T = -\log (I / I_0).$$

Absorption of light by a sample

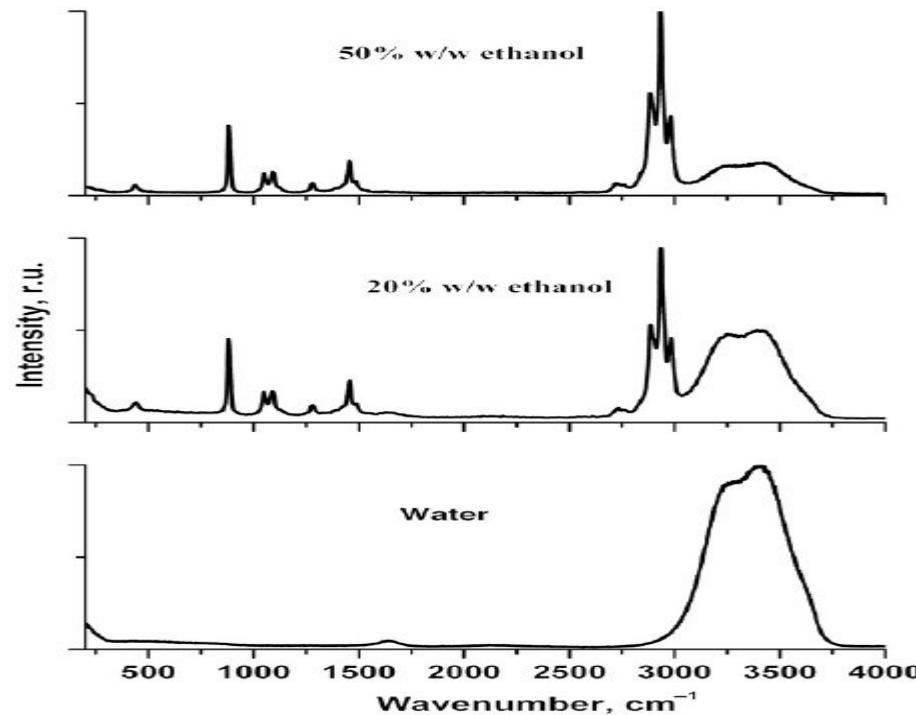


Modern absorption instruments can usually display the data as either transmittance, %-transmittance, or absorbance. An unknown concentration of an analyte can be determined by measuring the amount of light that a sample absorbs and applying Beer's law. If the absorptivity coefficient is not known, the unknown concentration can be determined using a working curve of absorbance versus concentration derived from standards.

La mole è l'unità di misura della quantità di sostanza.

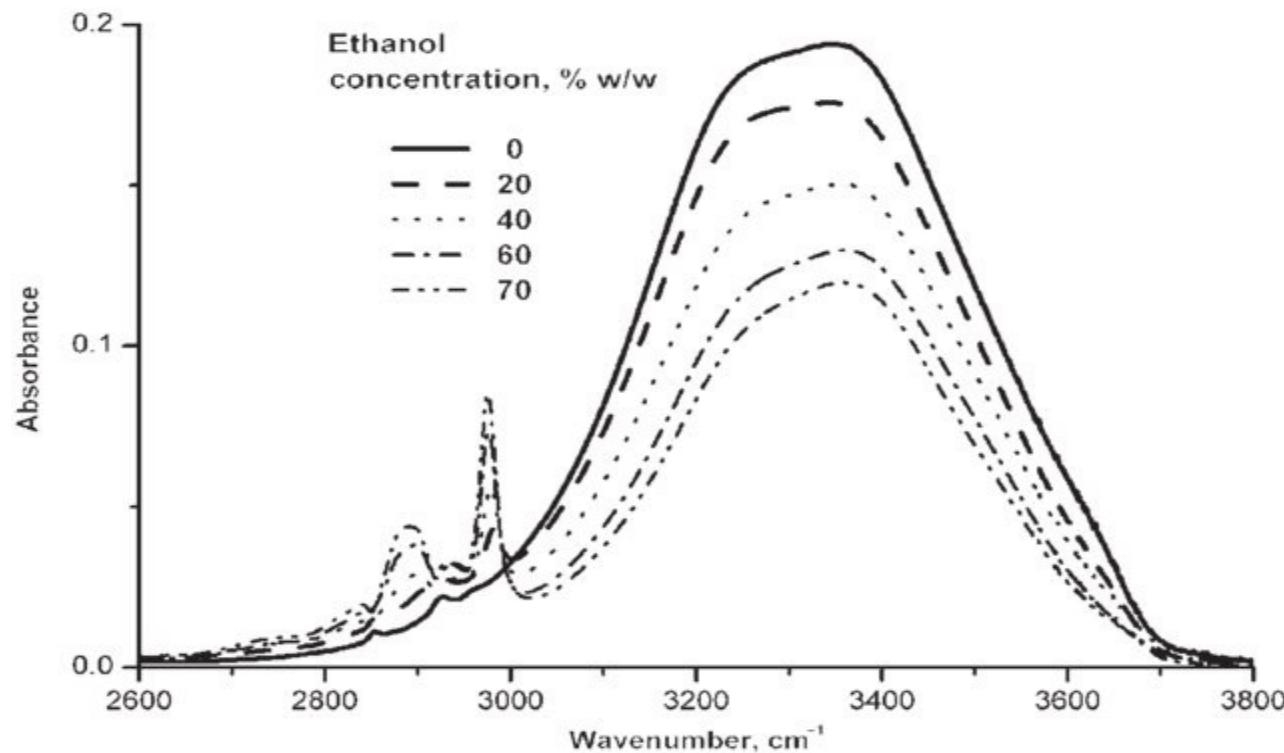


Spectrum Intensity distribution on water composite samples





Spectrum Intensity distribution on water composite samples





Spectrum Intensity distribution on water composite samples

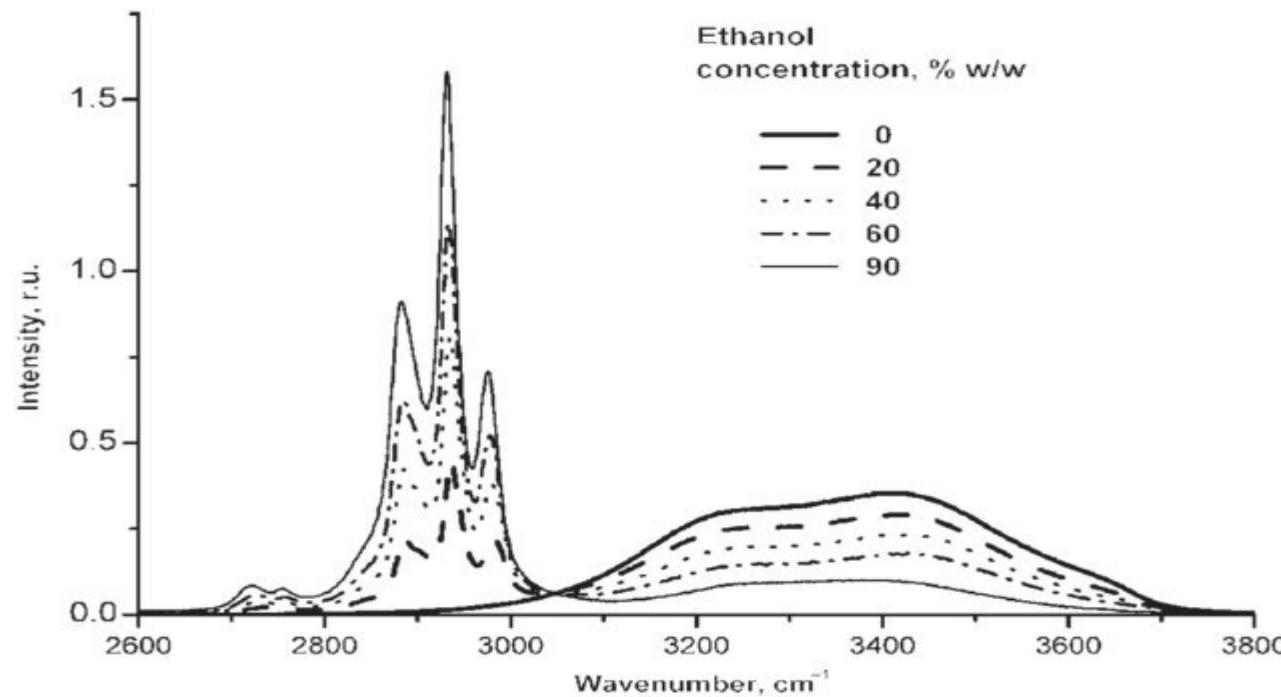


Figure . Raman scattering spectra of water and ethanol solutions with various ethanol concentrations within the region of CH and OH stretching bands.



Near Infrared spectroscopy

Some of the biggest advances in the food industry are being made possible by technological innovations such as

near-infrared spectroscopy, which can identify certain compounds like fat, sugar, water, and proteins in food, leading to information about calorie content, freshness, and quality of food that can help consumers make better choices. By analyzing the absorption spectrum of an unknown material and matching this measurement with a database of known molecules, it is possible to determine the presence and quantity of certain ingredients—for example, the percentage of cocoa in a chocolate bar.

La mole è l'unità di misura della quantità di sostanza.



Near Infrared spectroscopy

Quantitative and qualitative analysis

Infrared (IR) light stimulates the molecules in a material, causing them to vibrate; due to resonance, an atomic compound with a certain binding energy is stimulated by a photon with the same energy. Depending on the type of atomic bond, certain fundamental vibrations, harmonics, and combination vibrations can be measured in the IR range. A characteristic atomic connection thus occurs in several wavebands, depending on whether it is a fundamental or a harmonic vibration. In the near-infrared (near-IR), usually only harmonics are found.

In terms of food analysis, one of the goals is to determine the percentage of corresponding ingredients, such as sugar, fat, or water content. This method is called **quantitative spectroscopy**. However, in most cases, the object to be analyzed does not consist of a laboratory-pure mixture. As a result, the identification of the ingredients in complicated and unknown substances can be difficult to pinpoint because the individual oscillations can overlap in the overall spectrum. In contrast to the quantitative analysis mentioned above, this is a **qualitative analysis**. The mathematical models used here are much more complex and have to be geared to a reduced target quantity in order to achieve meaningful results.



On the path of mobile spectroscopy

As a result, there has not yet been a release of a handy spectrometer that consumers can carry in their pockets to get an immediate, detailed analysis of every piece of food they eat. Fortunately, however, the first steps toward this reality are now being made. In the near future, a mobile handheld spectroscope could ultimately be used to scan a wide range of materials—food, medicine, even the human body—and analyze them in real time.

A spectrometer consists of four main building blocks: a light source, a detector, optics, and a statistical mathematical model (so-called **chemometrics**)

[https://www.laserfocusworld.com/test-](https://www.laserfocusworld.com/test-measurement/spectroscopy/article/16562702/chemometrics-software-from-bw-tek-adds-new-algorithm)

[measurement/spectroscopy/article/16562702/chemometrics-software-from-bw-tek-adds-new-algorithm](https://www.laserfocusworld.com/test-measurement/spectroscopy/article/16562702/chemometrics-software-from-bw-tek-adds-new-algorithm)), which derives meaningful information from raw data.

The photoresponse of silicon-based detectors extends to just over 1000 nm; for longer wavelengths, sensors based on gallium arsenide are needed. The 780–1000 nm spectral region crystallizes out as a meaningful measuring range because it shows measurable characteristic curves for almost all key substances.



Chemometrics

Chemometrics is the science of extracting information from chemical systems by data-driven means. Chemometrics is inherently interdisciplinary, using methods frequently employed in core data-analytic disciplines such as multivariate statistics, applied mathematics, and computer science, in order to address problems in chemistry, biochemistry, medicine, biology and chemical engineering.

Chemometrics in Spectroscopy, Book • Second Edition • 2018

BWIQ is a multivariate analysis software package that analyzes spectral data to find internal relationships between spectra and response data or spectra and sample classes. It combines traditional chemometric methods like Partial Least Squares Regression (PLSR) and Principal Component Analysis (PCA) with a new proprietary adaptive iteratively reweighted Penalized Least Squares (airPLS) algorithm.

The case of compound water samples

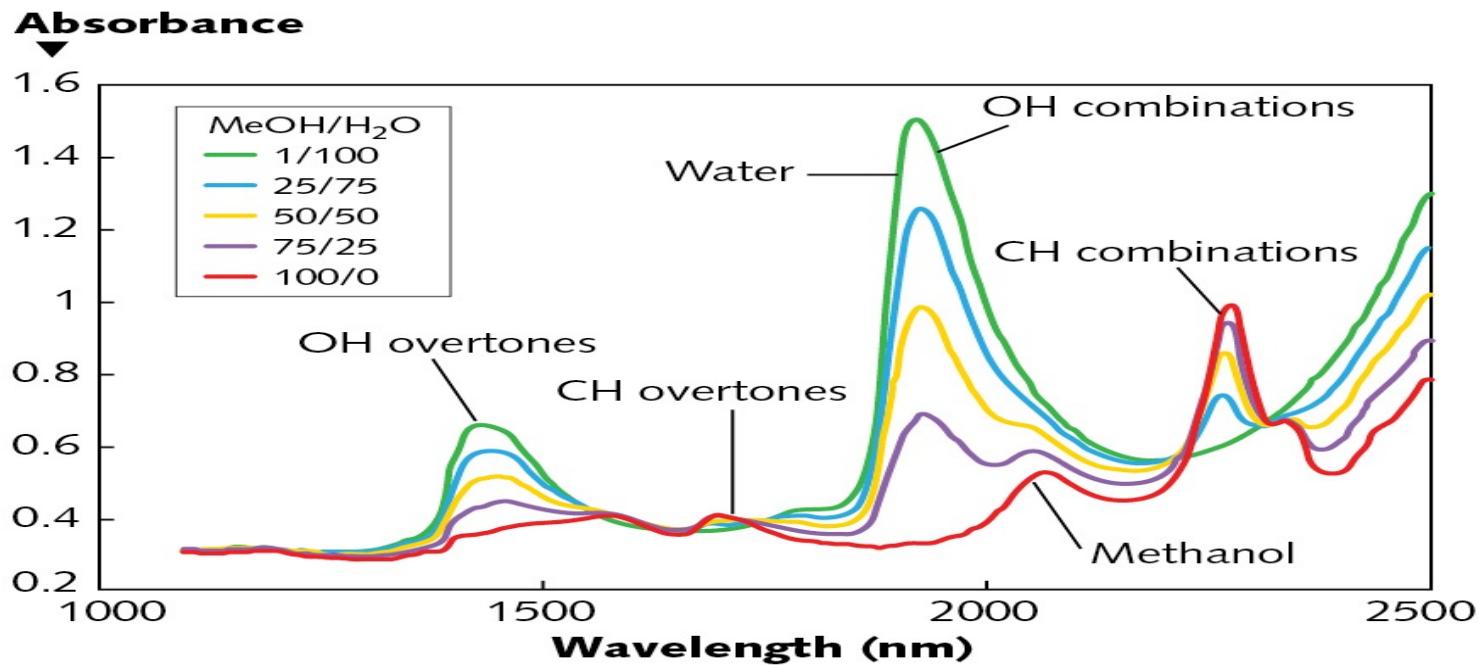
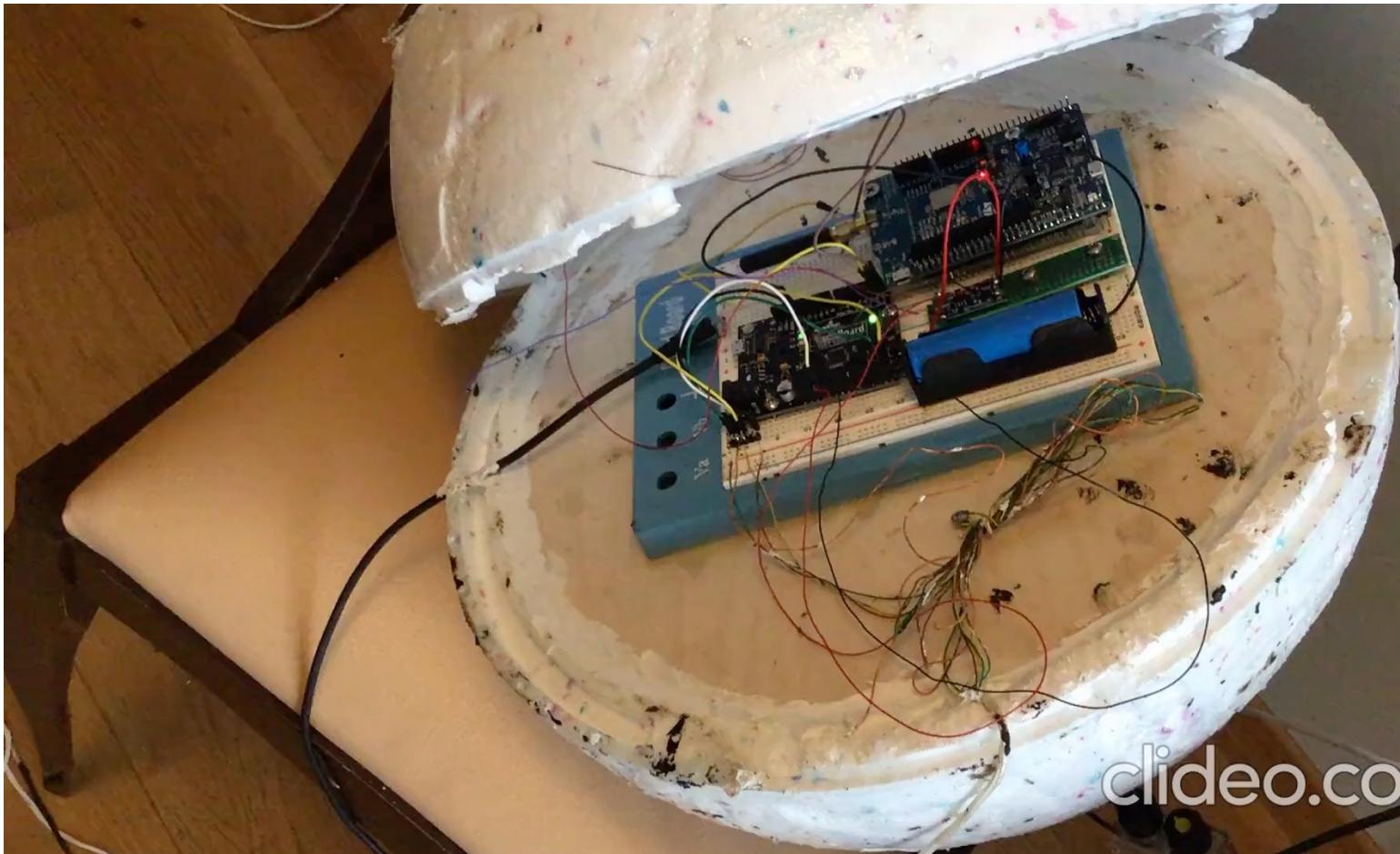


FIGURE 2. Absorption spectra of water and methanol under different mixing ratios.



The Smart Buoy at Work



clideo.com

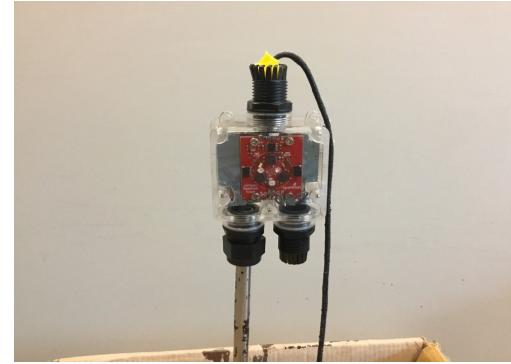
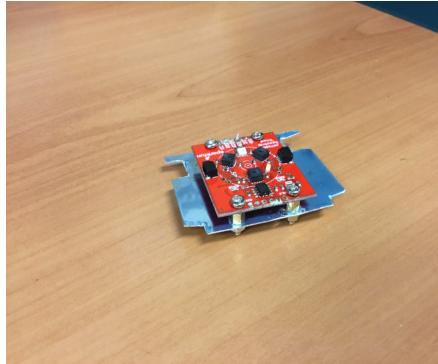
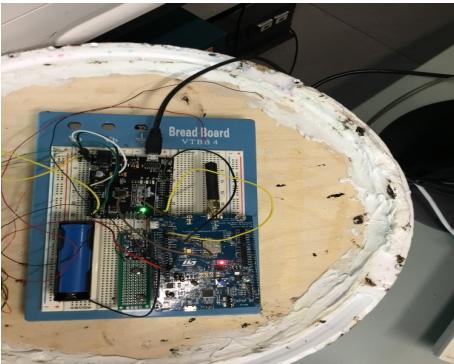


The Smart Buoy Sea Immersion





The Smart Buoy Components





Future Development

- Improve waterproofness of in vitro spectrophotometer
- Extend the model to other water quality parameters
- Refine machine learning module
- Improve anchorage system
- Improve connection and data transfer from Arduino to B-L072Z-LRWAN1
- Connect B-L072Z-LRWAN1 with IC880A LORA Concentrator
- **Other**

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Grazie per la Vostra Attenzione!



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