REPORT: Final project. High-fidelity, low-budget, 3D-printed spectrophotometer.

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Abstract.
A cheap 3D-printed spectrophotometer was assembled and tested against a commercial device in order to tests it's reliability. From the test, different conclusions are reached concerning the device's usefulness and limitations. It was determined that the 3D-printed device works very well as a tool for teaching the basics of spectroscopy to undergraduate, high-school and even middle-school students. A MATLAB application was also developed to make the interpretation of those images taken even more accessible. It was hoped by the team this would be the genesis for a future cellphone "app".

I. INTRODUCTION

Absorption spectroscopy is an experimental approach commonly used to measure the concentration of colored compounds in a sample. UV-Vis spectroscopy has a wide array of applications in chemistry labs such as nanoparticle characterization [1] and kinetic-equilibrium studies of reactions [2]. Given its importance, it is then desirable to be able to use spectrometers for educational purposes in most undergraduate chemistry labs, having as the biggest obstacle the high-cost nature of this equipment.

An absorbance spectrophotometer compares the intensity of light across the visible spectrum in the presence and absence of a sample. In general, a white lightsource is directed through a sample and then a diffraction grating in order to see the visible range spectrum. For the case without a sample, the light passing through the device would have measured wavelenght dependent intensity $I_0(\lambda)$. When the sample is in place light would be absorbed in specific wavelenghts depending on the color of the sample, giving as a result an intensity profile $I_s(\lambda)$ [3].

Transmission at each wavelenght equals the amount of light at each wavelenght that went through from the original spectrum. This can be expressed as equation 1 and absorbance is then defined as equation 2.

$$T = \frac{I_s(\lambda)}{I_0(\lambda)} \tag{1}$$

$$A = -log_{10}(T) = log_{10}\left(\frac{I_0(\lambda)}{I_s(\lambda)}\right) \tag{2}$$

With the use of the Beer-Lambert Law in equation 3, concentration can be measured from absorbance if absorptivity and path lenght are known. Thus, under similar circumstances absorbance could be measured from concentration as well.

$$A = \epsilon(\lambda) \cdot l \cdot c \tag{3}$$

The team's objective is to use the 3D-printed spectrophotometer design used by [3] and create a program that would do the image processing with minimal input from the user. This feature will make use of a wi-fi connection to send the images from phone to computer, where images would be processed in a matter of a couple of minutes and graphs would be displayed to the user without the need to have any programming background. This in contrast to other similar projects where an image processing software such as ImageJ was used [3].

Expected results include intensity and absorbance graphs as a function of wavelength for different concentrations of green food coloring. Using absorbance information for different concentrations then it is expected that a linear regression will yield information of absorbance for determining unknown concentrations and vicecersa [4]. Results will be compared with those of a dedicated commercial UV-vis spectrophotometer in order to have and idea of the fidelity of the 3D-printed design.

II. EXPERIMENTAL PROCEDURE

A. Construction of 3D-printed spectrometer

The Elise K. Grasse *et al.* design for the case was downloaded online and printed using a 3D printer with standard filament. As the only optical property relevant for our experiment is intensity a cheap commercial mirror was used and applied into the case. A diffraction grating was retrieved from the school's Physics Department and set by the base were the cellphone rests as shown in Fig. 1 (obtained from [3]).

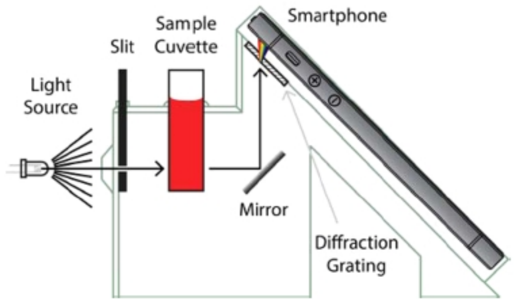

FIG. 1: Diagram of the arrangement of the SpecPhone device as designed by [3].

The data acquisition device of the 3D spectrometer is an iPhone 5 camera (8 MP) whose photos are 3264x2448 pixels, has a IR filter, and spatial noise reduction. This last will surely affect the obtained spectrogram. A purple glow may appear when in presence of a strong intensity source (lens flare). This may be due to the sapphire lens and is a common issue of digital cameras.[5] Our light source is a common white LED.

B. Concentration determinant solution

The sample solutions were prepared with green food coloring and distilled water in proportions 0.00625%, 0.0125%, 0.025%, 0.5%,and 1%. First the 1% was prepared in a 50 mL beaker as a "stock" solution. The later solutions where obtained by diluting the stock with distilled water. The reasoning behind the preparation of this solutions is to be able to track the change in absorbance as concentration changes.

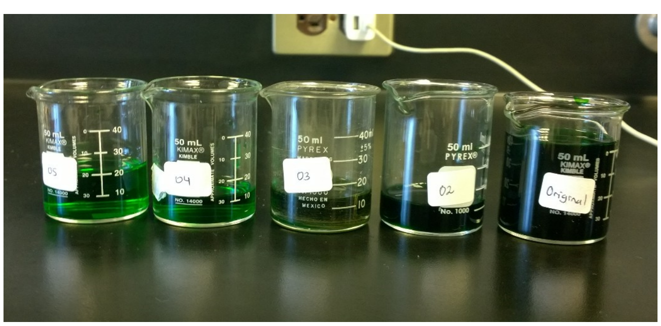

FIG. 2: Solutions for the following concentrations of green dye in distilled water. From left to right: 0.00625%, 0.0125%, 0.025%, 0.5%, 1% (Stock solution).

C. Data acquisition

Data is acquired from the SpecPhone camera directly and sent via wi-fi to a computer were an app is ready to make analysis.

D. Data analysis (Specphone App)

As an addition, an image analysis application was developed using MATLAB software.

The principal focus of the SpecPhone app is centered in the calculation of intensity and absorbance profiles for each of the samples taken, but it can be also used for reaction kinetics analysis.

Explanation of the processing order is as follows:

1. Directory browser : Images get imported into an specified folder and prepared for analysis.

2. Analysis preparation: Pictures for either the reference and the sample to be analyzed are displayed. The X slider and edit text panel are used to specify the pixel column to analyze. The Y edit and graph length parameters specify the pixel start and finish numbers from the chosen column.

3. Processing: Intensity profile comparation between the sample and the reference and their absorbance measure based on equation 2. All graphs are normalized to make comparison easier between the other spectrometers. Y label are arbitrary units and X label is wavelength. Wavelength calculation is done prior to the analysis and implemented internally. In this case, wavelength range is the full visible spectrum (400-700). Wavelength increments are based on picture resolution. It is important to identify both spectrum limits on the image to obtain a coherent mapping.

4. Annotations : Posterior to analysis, user can arbitrarily choose which measurements are good and redo those which weren't good enough. Values such as intensity and absorbance profiles, average absorbance and sample concentration are saved. Concentration and average absorbance are displayed within the app for quick check-up.

5. Regression / Stacking : After experiment is done, the regression button performs simple processing for an easier comparing visualisation (figures 4 and 5). A moving average smoothing can be applied to reduce noise from the input. In this case we use a moving average of a 10 pixel window.

6. Output: Analysis output and stack plots for absorbance and intensity profiles can be saved in matlab format using the app. Information about the experiment containing raw intensity and absorbance profiles, reference image and analysis coordinates are also included.

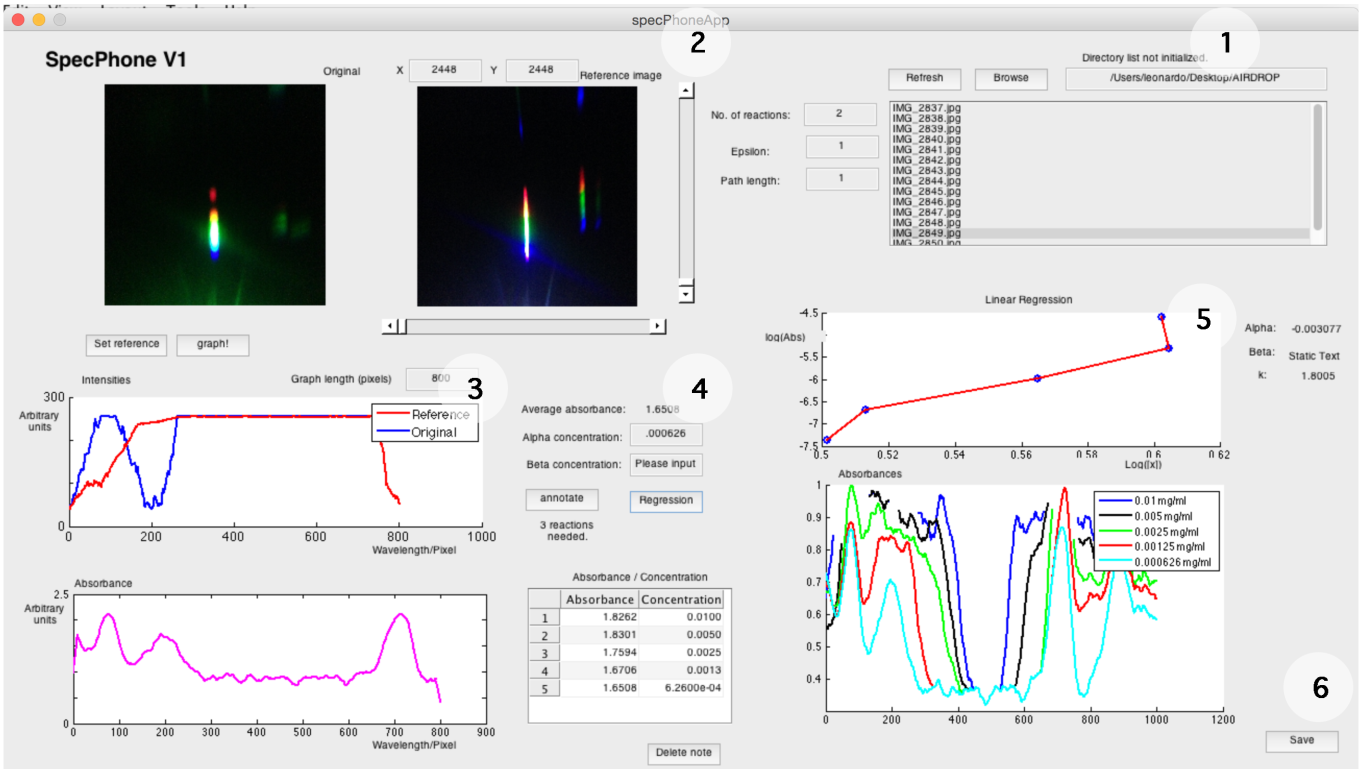

FIG. 3: Graphic Interface of Specphone App where image processing is reduced to choosing the position of the vertical axis where the image will be analyzed. Results displayed include intensity and absorbance graphs as well as a linear regression of the data analyzed.

Specphone app code is freely available in https://github.com/LeonardoClemente/SpecPhoneApp

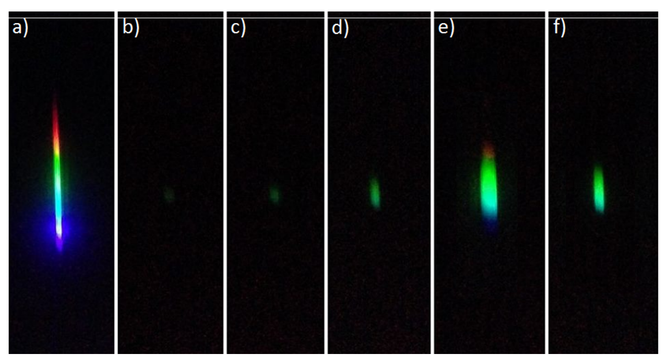

FIG. 4: Images obtained with SpecPhone prior to processing. Samples used: a) distilled water; solutions of green dye in concentration b) 1%, c) 0.5%, d) 0.25%, e) 0.125%, and f) 0.0625%

III. RESULTS

Using the SpecPhone a spectogram of each substance was obtained. A collage of all these JPG images is shown in Fig. 4. In this figure it's very apparent how greater concentrations of green dye cause a more opaque profile where absorption should be greater and perceived intensity smaller.

In the MatLab application, equation 2 was used, making it possible to obtain both an intensity and absorbance normalized profile for each cellphone spectrogram. These are shown in Fig. 5 and Fig. 6 respectively.

For device calibration it was suggested by [6] that lasers with a know dominant wavelength should be used. However, due to equipment limitations the approach suggested by [7] was preferred, where a rough estimate of the wavelength was chosen for two pixels in the reference picture (picture a) in Fig. 4) and from there the pixel distance was equated to a wavelength difference.

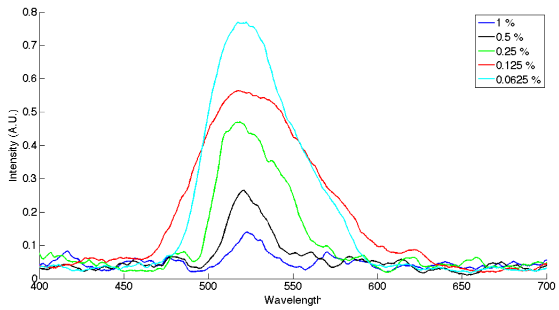

FIG. 5: Intensity profile obtained with SpecPhone graphed against wavelenght for the following concentrations: a), b), c), d), e)

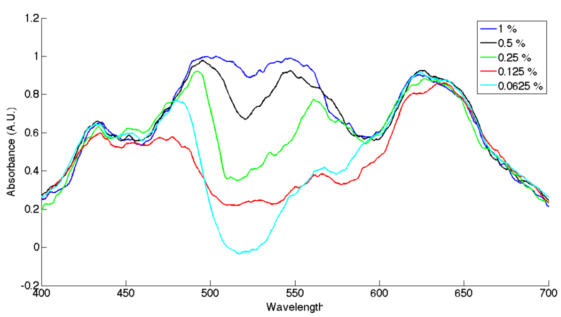

FIG. 6: Absorbance profile obtained with SpecPhone graphed against wavelenght for the following concentrations: a), b), c), d), e)

Results in Figs. 5 and 6 correctly show a peak perceived intensity increment with lowering concentration. The lowered opacity not only causes the green intensity peak to increment but also other colors to be more apparent, which was obvious in Fig. 4.

Figs. 7 and 8

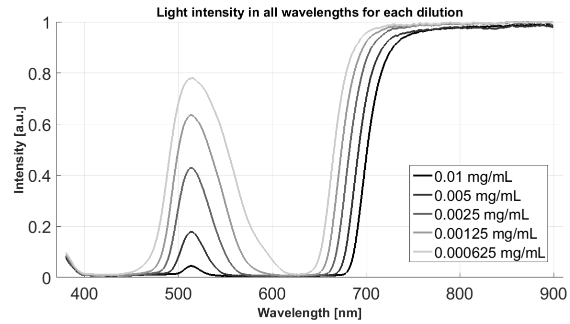

FIG. 7: Diffracted source light profiles according to a), b), c), d), e) samples analyzed with SpecPhone

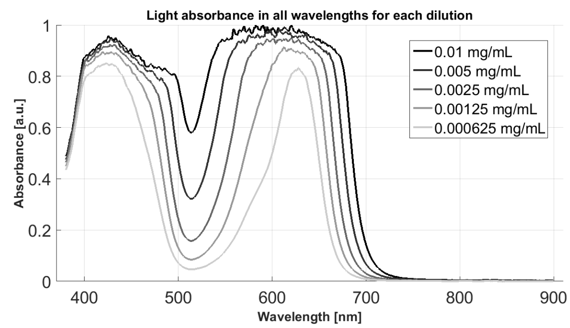

FIG. 8: Application developed to help in spectroanalysis.

A linear regression was performed with the data according to concentration. Results are shown in Figure 5 where a total of NUMERO data pairs were used.

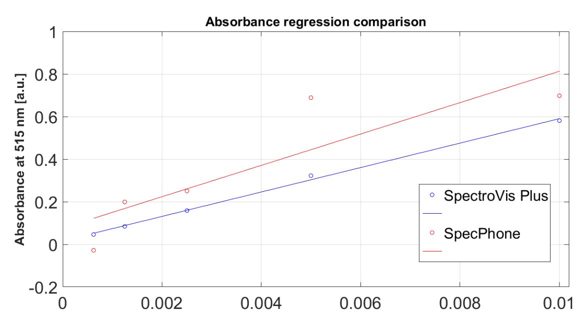

FIG. 9: Linear regression of both SpecPhone and SpectroVis Plus measurements for absorbance at 515 nm. R^2 values for each of them are0.8746 and 0.9987 respectively.

IV. DISCUSSION

The differences between the 3D-printed spectrometer and the commercial one are readily apparent. This was also reported by [4], were a greater range of spectrometers were compared. Results given by the SpectroVis Plus device are considerably smooth and clear (Figs. 7 and 8), while those taken from the iPhone appear noisy (Figs. 5 and 6). Concerning this, it should be considered that the MATLAB application already performed an "smoothing" operation.

It must be noted that the iPhone 5 camera is not one that is designed to take these kind of pictures, but rather pictures that would look good to the user. The phone's camera auto-sets exposure, which makes intensity quantification difficult. It then saves pictures in the compact but lossy JPG format, which blurs the image. Also, it's also easily seen that the cellphone spectrometer is unable to measure the intensity of IR frequencies. This probably has to do with the IR blocker most digital cameras have, since without it the red channel would be oversaturated.

During the performance of the experiment, intensity saturation was a big problem. This was warned upon by [7], where a different DIY spectrophotometer device with similar purposes was constructed and tested.

The absorbance regression comparison between the data obtained with the SpectroVis Plus device and the cellphone spectrophotometer (Fig. 9) shows that the both R^2 are quite close to each other. Differences between them may have arisen because of residual stray light or automatic correction made m This is a similar result to that obtained by [4].This shows that while not perfect, the device fulfills it's intended role.

As noted in [3] and [7] cellphone applications for spectroscopy already exist, but they are unreliable or require considerable more equipment or a more complicated arrangement than that used currently. The current device and MATLAB application allow for a very acceptable and easy evaluation of data.

V. CONCLUSION

In this paper we've reported on the capabilities, possibilities and quality of a DIY spectrometer: the SpecPhone. As it has been shown, the cellphone spectrophotometer is inadequate for routine analysis, but a very cheap and accessible tool to teach spectroscopy concepts to students.

It was determined that results obtained by both the SpecPhone and a commercial spectroscopy device are of comparable quality. At least for the visible range, normalized and absorbance graphs appear quite similar, while the regression analysis gave surprisingly accurate tendencies. Therefore, it works in order to teach concepts of concentration vs. absorbance/intensity.

The MATLAB application proved very useful to process image data into intensity and absorbance profiles, regressions and comparisons between data sets. This allows the student to do measurements and analysis on their own with little or no knowledge in programming.

The team believes that given the proliferation of smartphone devices today, that the development of a dedicated smartphone app is obvious next step Hopefully this work will push development into that direction.

VI. REFERENCES

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