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3D Printing Applications within Spectrophotometry

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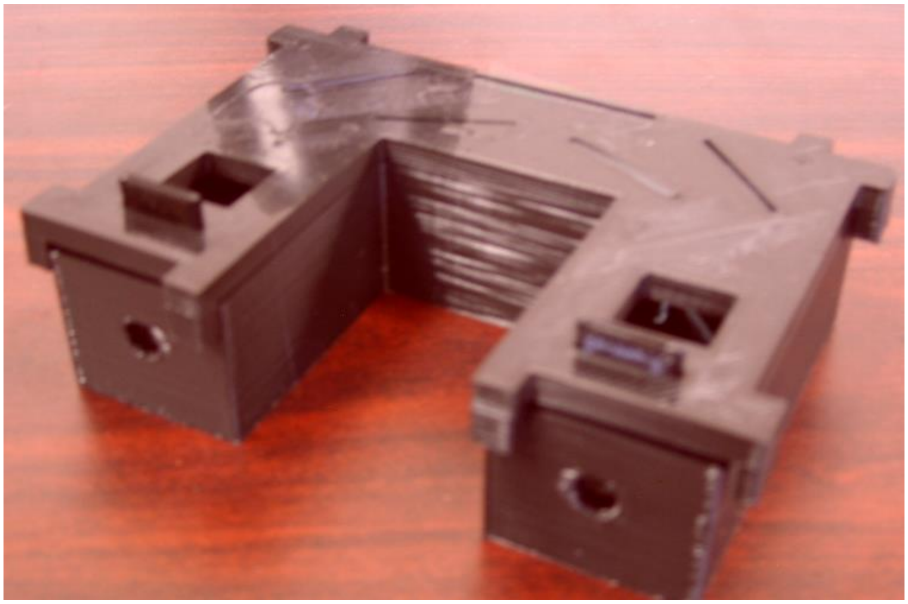
Abstract

Ultraviolet-visible spectroscopy is a tool used throughout the field of chemistry and in chemical labs across the world. Spectrophotometers are a core technology in analytical chemistry, and are used to obtain accurate data on solution concentration. Unfortunately spectrophotometers can be difficult to obtain due to their high cost and low availability outside of a laboratory; this is especially true in either high school or lower grades where buying a spectrophotometer could be considered unreasonable due to price. There are ways to obtain cheaper spectrophotometers, but they can have a high initial cost or low overall quality. This paper will discuss and present a 3D printed spectrophotometer that is inexpensive to build, but displays an overall quality that will allow for accurate measurements of analyte. The design is relatively simple and allows for one time placement of both a blank and analyte cuvette, which makes for a more convenient and time efficient measurement.

Abstract Graphic



Keywords

Ultraviolet-Visible Spectrophotometry, Analytical Chemistry, 3D printed, Analyte, Cuvette

Introduction

The principal of Ultraviolet-Visible (UV-Vis) spectroscopy is the measurement of light absorption as it passes through a material and provides information about the electronic transitions that happen within the sample. With these measurements one can then determine the concentration of a sample using Beer's Law which relates absorption of light as it travels through materials. UV-Vis spectroscopy can also allow for these electron transitions to be characterized as indirect or direct and if it is allowed or forbidden, however this is a more advanced technique and will not be addressed within this paper.[1] Spectroscopy is not just a simple tool to be used in educational setting, but is applied in everything from environmental protection to composition of heavenly bodies.

UV-Vis spectroscopy can be used to identify the concentration of analytes within a solution. A recent example of this is a group of scientists studying the wastewater from a paper mill treatment plant.[2] In this study the group used a submersible UV-Vis spectrometer that allowed for measurements in real-time of the wastewater's pollutant contents. This spectrometer was reasonably advanced due to it being able to operate underwater, utilizing the whole range of UV-Vis (200-750 nm), and having an auto-cleaning system that prevented the growth of films on the device. The results of the paper revealed that the instrumentation allowed for proper operation and control of the waste treatment plant.[2-4]

Spectroscopy is not limited to applications within our planet, and has been used to obtain the chemical composition of the Orion nebula. This study not only helps to show the diverse uses of spectroscopy, but the variety within spectroscopes due to this study using echelle spectroscopy. At its core echelle spectroscopy is much like other diffraction gratings in the fact that it contains slits that have a close width to a wavelength of light that has been diffracted, but is different in the fact that having longer wavelengths overlap with shorter is wanted and used. This is accomplished by mounting another grating or prism into the beam path allowing for accurate measurements to be taken. Scientists have used this class of spectroscopy to observe the nebulas, quasars (young galaxies), and even brown dwarfs (objects that are too small to be a star, but too large to be a planet).[5-9] This study enforces the fact that spectroscopy can be utilized in a wide range spanning from the study of vast bodies within the universe, to introducing high school students to the concept with a 3D printed spectrometer.

3D printing is an emerging tool within chemistry, as well as many other scientific fields, which applications and promise are immense. For this project a spectrophotometer was 3D printed, tested, and uploaded online to provide a cheap alternative to obtaining a spectrophotometer. Spectrophotometers can cost thousands of dollars limiting those who have access to them, specifically those outside of a laboratory environment. As explained spectroscopy is a crucial portion of chemistry and could be introduced at earlier points in a student’s education so that when they enter college or a laboratory they are familiar with the concept. Uploading this design to a website such as Thingverse enables individuals to print their own spectrometer while only needing access to a 3D printer for a short period of time.

3D printing is a new technology that could revolutionize the way that research and teaching is performed within laboratories. With recent advances within the technology this device has become more widely available, efficient, and affordable. Roles have been found within an industrial setting being used for printing prototype parts for planes and cars, building models, and even in development of consumer products. This reach of influence extends even to the manufacturing and prototyping of weapons for the military, prosthetic limbs, food, and fashion.[10-13] For this project the 3D printer was used to design and print a functional spectrophotometer, which was used throughout the experiment.

Principal

Spectrophotometry's core concept is to measure the intensity of light across the visible spectrum as it passes through a sample, and a blank. A blank is a cuvette filled with a solution that does not absorb any of the wavelengths of light, and allows for a full spectrum to be measured. Typically white light passes through a slit, proceeds to pass through a sample, diffracts through the diffraction grating, and has a picture of the spectrum taken by a camera.

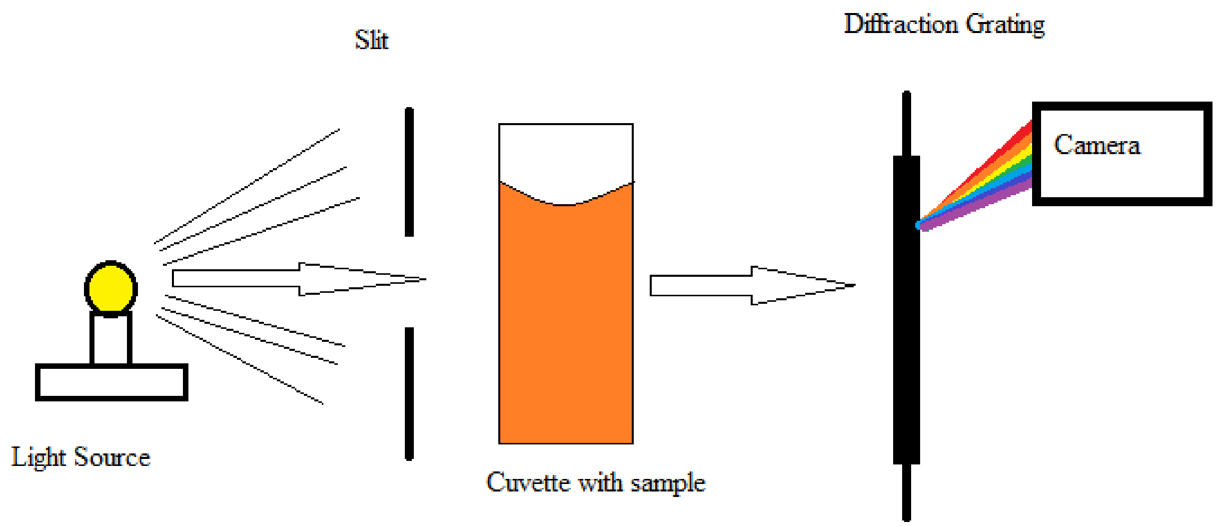


Figure 1: Light is produced form the light source and travels through the slit to allow only a controlled amount of light to pass through the sample. The light then passes through the diffraction grating causing dispersion of the light and travels into the camera allowing for analysis of the sample. The camera in this case was that of an Iphone® 5.

This whole process can be summarized by two equations, the first of which is the equation for Absorbance:

$$A = -\log(T) = \log(\frac{Io}{\mathrm{Is}})$$

where *A* is the absorbance, which is the negative logarithm of the transmission, *T,* that can be found by taking the logarithm of the wavelength measured with no sample in place ,I_o, divided by the wavelength resulting from the light passing through the sample, I_S. The Beer-Lambert law also denotes how to measure absorbance with the equation.

$$A = \varepsilon \cdot l \cdot c$$

In this equation the absorbance is denoted by *A* and is equal to the molar absorptivity, ε, multiplied by the length of the light path that the light travels through the sample, *l*, multiplied by the concentration of the sample, *c.*

3D Printing

The project began with the drafting and designing of a spectrophotometer with the program Solid Works. Several designs were drafted and discarded before the final design was used, which is pictured above in the abstract. The final design can be described as a dual sided UV-Vis spectrometer, which uses mirrors to allow for the measurement of a blank and a sample without having to switch out the cuvette.

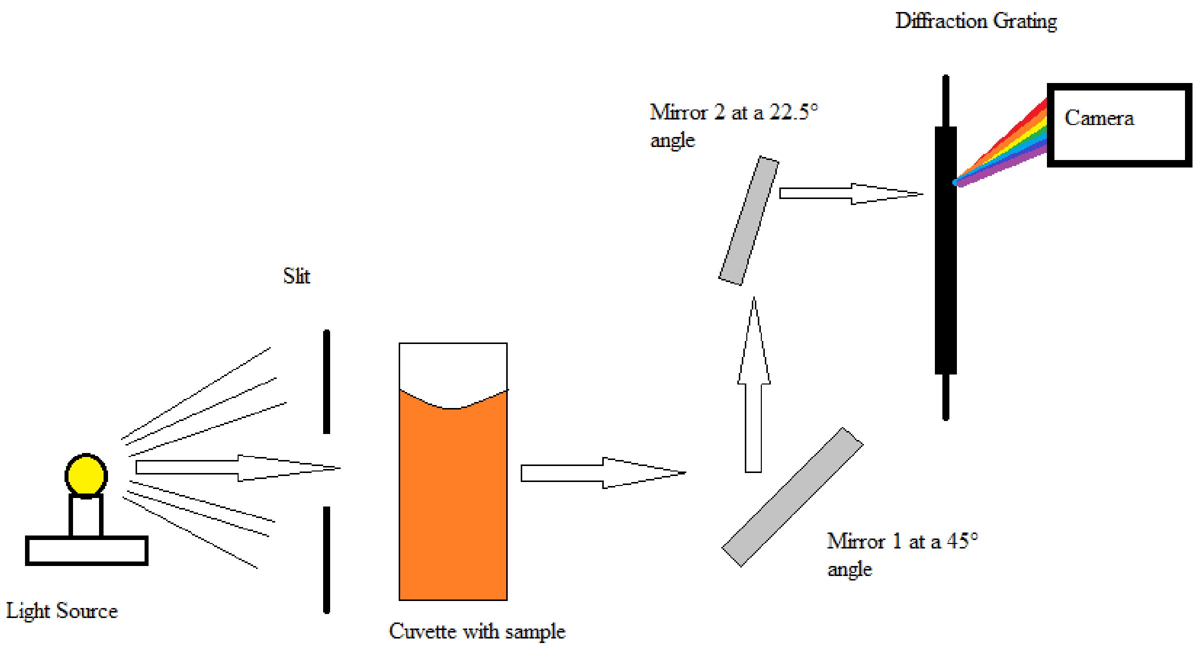


Figure 2: One side of the spectrophotometer developed. It is similar to the basic spectrophotometer except for the 45° angled which allows for the light to bounce in a straight line at mirror 2. The second mirror is at a 22.5 ° angle to allow for the light to strike the diffraction grating to allow for a measurement of the full visible spectrum. Note that this is the set up on both arms of the spectrometer.

Key Features

Some of the more important aspects of this spectrophotometer come from the inserts that are used to ensure that the design will work as a spectrometer. The inserts were printed as separate pieces and were roughly 38.1 millimeters long, with a slit approximately 1.27 millimeters in width. This piece controlled the amount of light that would pass through the sample and be measured.

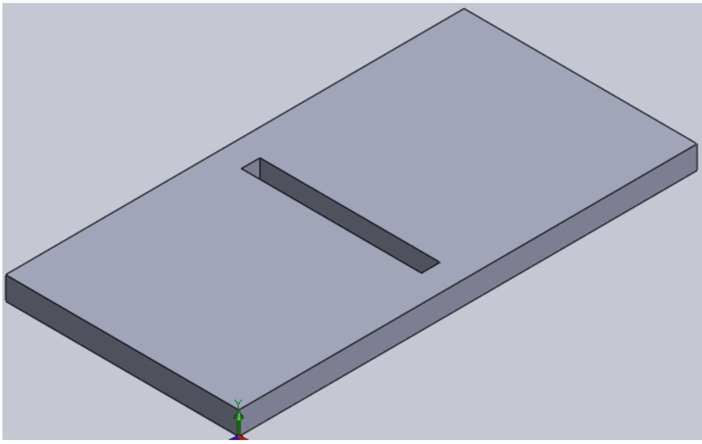


Figure 3: The slit that was 3D printed and inserted into the spectrophotometer. The slits measurements are 38.1 x 15.24 x 1.524 mm and a slit of 1.27 mm.

The top of the spectrometer was also designed to have two cuvette holders to allow for the placement of cuvettes with a base of 1 x 1 cm.

As shown in Figure 2 mirrors were needed to direct the light to the diffraction grating allowing it to disperse properly to the camera. In this instance the mirrors were 1 x 1 inch aluminum mirrors, four of which were used. The first mirror rested at 45° to allow for the direct transmission of the light to the second mirror positioned at 22.5°, which allowed for the dispersion of light through the diffraction grating into the camera.

The diffraction grating was a film sheet with 1000 lines/mm and was cut with scissors so that it could fit into the designed slit within the spectrometer. A diffraction gratings purpose is to refract light through a series of lines that are parallel at varying densities depending on the grating. The light source used and shown through these parts came from a handheld pen light, but could be replaced with any white light source such as a desk lamp or LED.

Assembly of the spectrophotometer was something that evolved over time with this project. Initially the spectrometer was one solid design, but because of the limitations of the 3D printing software the top would sink causing distortion and alter its dimensions. Therefore, it was split into two separate pieces a bottom with the channels through which everything could be placed and light could travel through, and a top with slots that would hold all of the aforementioned pieces.

Applications

The main use of this 3D printed spectrometer would be for introduction into the field of spectrophotometry rather than acting as a standalone piece of lab equipment. To this end, and due to time restraints, the device was tested with a portion of the experimental procedure found in Dr. Smith's lab at the University of Akron. This experiment has a student using Kool-Aid® mix to create solutions with different concentrations, measure the visible light spectrum, and compare the results. This goes well with the idea that this device will be used to introduce the concept of spectrometry. For the testing three separate measurements were taken of a solution at varying dilutions. The first dilution, A, was 0.2 grams of Kool-Aid® orange mix within 100 mL of water, and the second, B, was 5 mL of the A solution diluted with 5 mL of DI water, and the final measurement was simply DI water known as the blank.[14]

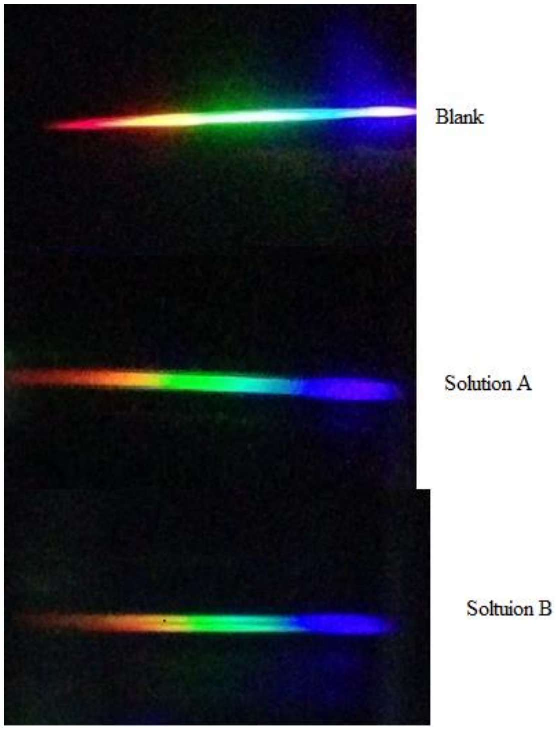


Figure 4: Pictures taken of the blank as well as solution A and B with the Iphone 5®. These were the pictures then used to analyze and obtain the graphs in figure 5. Note that the blank is more intense than sample A or B because of having no particles within the solution to absorb light.

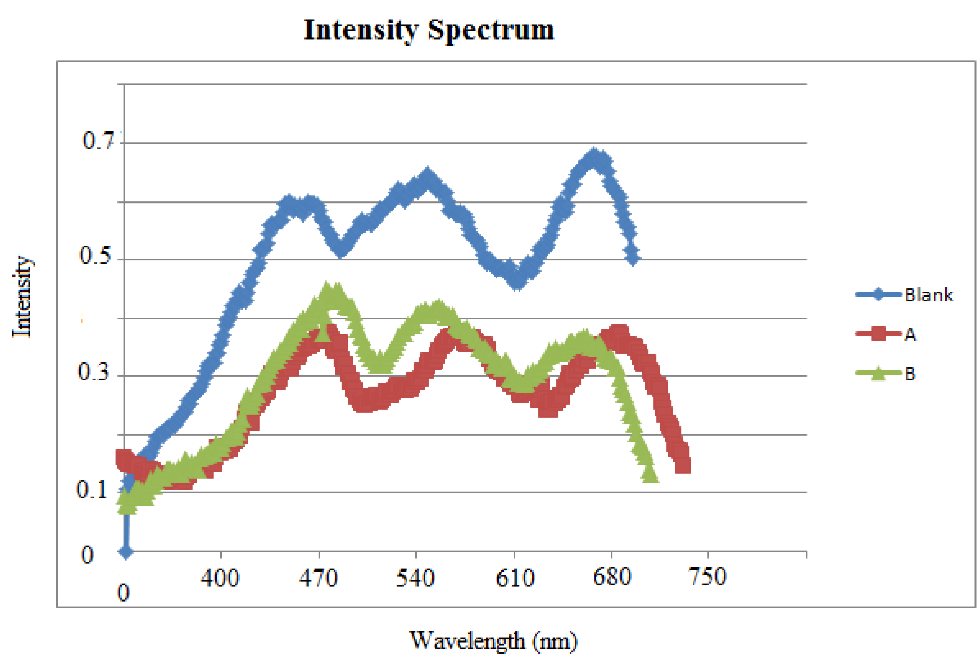


Figure 5: Using the program ImageJ and Microsoft office excel the following graph was obtained. The results show a clear distinction in absorbance between the blank, solution A, and solution B due to the intensity of the light in each line. The blank line is the most intense because it has no particles within it to absorb light. Solution B is more intense than solution A because it is a more diluted solution and has less particles to absorb light.

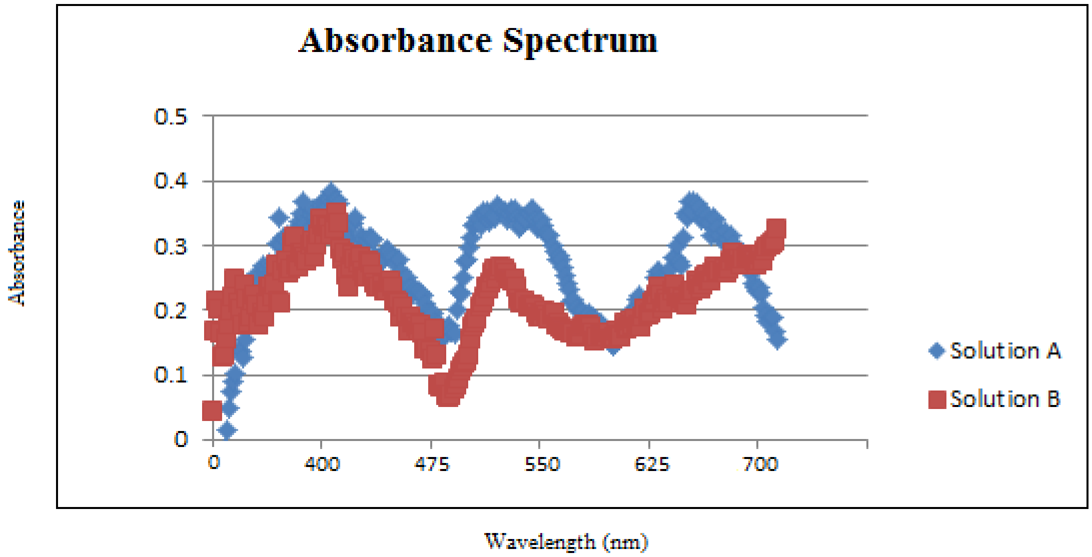


Figure 6: Using the Beer-Lambert Law of $A = -\log(T) = \log(\frac{Io}{Is})$ the absorbance of Solution A and B were found. The equation was used within excel to calculate all of the points on the graph. Analyzing the data that was collected shows that solution A absorbed more of the light passing through than solution B. This is explained by solution A being more concentrated with the amount of orange Kool-Aid® and therefore having more particles within it than solution B to absorb the incoming light.

Conclusion

The results obtained from measurements of the blank, solution A, and solution B support that the 3D printed spectrophotometer can produce accurate spectrums. Analyzing the intensity graph that the data produced shows that the blank had the least amount of light absorbed due to the higher intensity peaks and brighter image from the camera itself, solution A had the least amount of intensity due to it containing the highest concentration of orange Kool-Aid® mix, and solution B had a higher intensity than A due to it being more diluted than A. The absorbance graph followed this pattern of solution A having a higher absorbance than solution B, confirming that solution A was more concentrated and therefore had more particles absorbing light as it passed through the cuvette. The next steps within this project would be to obtain more results to ensure accuracy, and if this was accomplished to design more attachments for the spectrophotometer such as a phone holder to help with more consistent pictures. Along with this small tweaks could be made to the overall design such as a cover for the top of the spectrophotometer to filter out even more ambient light. Overall, this project has had a good start and can be used to create a quality spectrophotometer for the purpose of introducing the concept to individuals.

Safety

No hazards are associated with the assembly of the spectrometer, as well as the experiment performed to test the device. The printing of the spectrometer has a minor hazard within the extruder on the device that heat up to 220° C. Should an experiment be used in conjunction with this device and the solution being measured is unknown standard laboratory safety guidelines should be addressed. This would include items such as safety glasses and gloves being worn at all times.

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