Concentrations of Dyes in a Mixture

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AP Chemistry

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Introduction:

The color given off by any substance is determined by the wavelength of its electromagnetic radiation. However, visible wavelengths are only a small subset of all possible wavelengths as the human eye can only detect wavelengths from 400 to 700 nm. These wavelengths can be absorbed as it passes through substances which are measured as absorbance. Spectrophotometry is a laboratory technique which quantitatively measures the wavelength of electromagnetic radiation of a substance using absorbance. Transmittance is defined as how well a substance can pass light through itself. Absorbance and concentration is related by Beer's Law: $A = \epsilon l c$ "where A is the absorbance, ϵ is the molar absorptivity constant (which depends on the chemical species, wavelength of light and other things), l is the path length in centimeters, and c is the concentration of the solution" ("Experiment 10.1", 2019). The purpose of this lab was to determine the concentration of dyes in an unknown mixture by quantitatively measuring the wavelengths and absorbance of known mixtures with its concentrations using spectrophotometry. The concentration of the unknown mixture was predicted by constructing two different models: nonlinear regression and system of equations.

Materials:

- Vernier SpectroVis Spectrophotometer
- Cuvettes
- Computer with Graphing Software
- Deionized Water
- Solutions of Varying Colors

Procedure:

2.5 mL of solutions of varying colors and concentrations—blue, red, yellow, green, and an unknown mixture—were transferred to cuvettes. By using a spectrophotometer, these solution's absorbances were measured. This data was then transferred to a computer with graphing software and analytical tools.

<u>Results:</u>

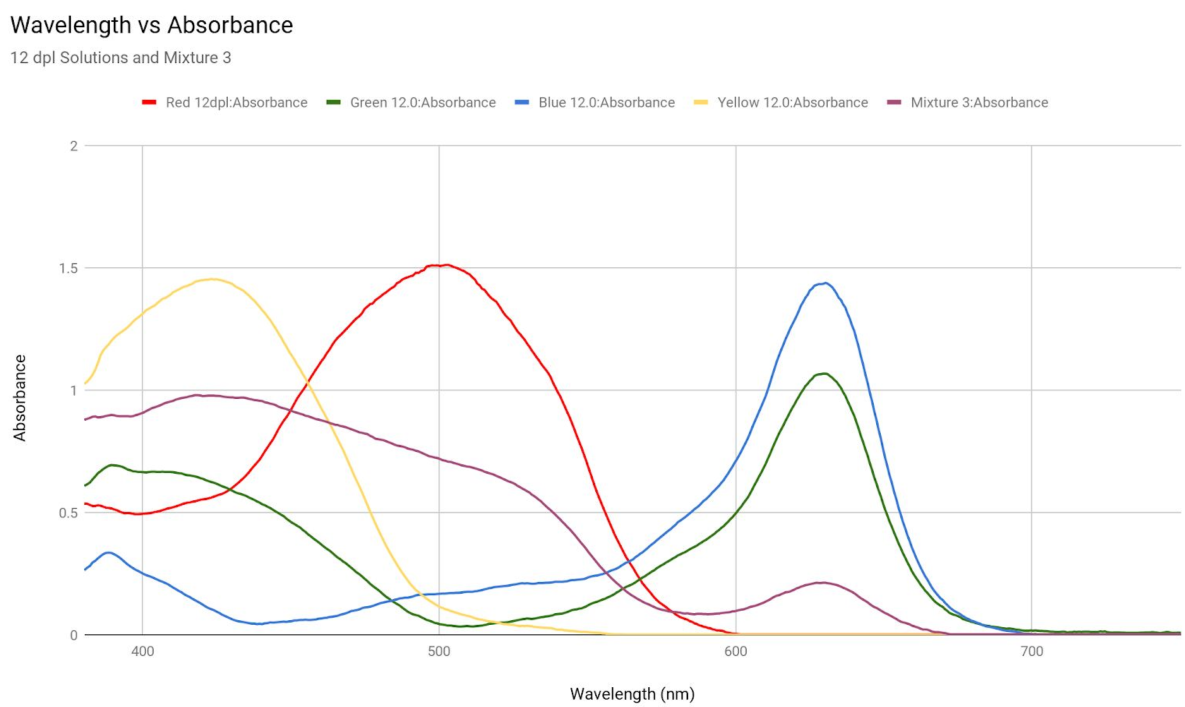

Figure 1 Relationship between wavelength and absorption of 12 dpl (drops per liter) solutions of differing colors and unknown mixture 3.

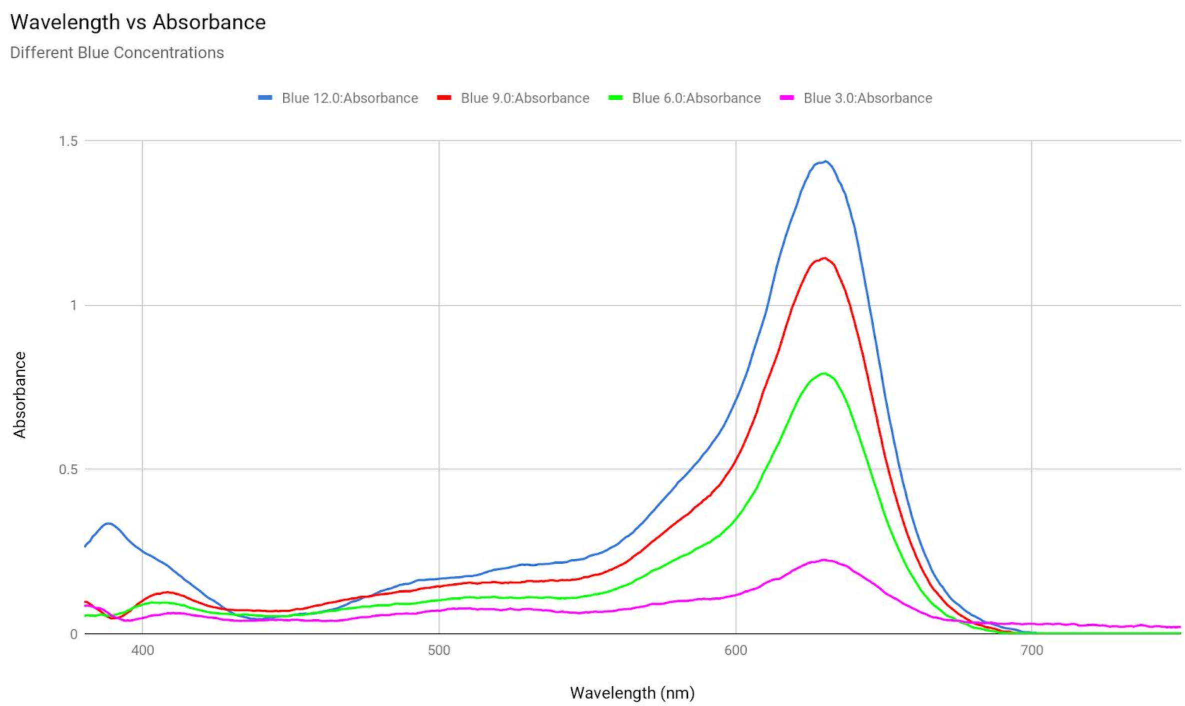

Figure 2 Relationship between wavelength and absorption of varying concentrations of blue.

Analysis:

It was given that mixture 3 was a combination of red, blue, and yellow solutions. Thus, mixture 3 was modeled as a function of wavelength:

$$f(\lambda) = A_{m(\lambda)} = \rho\, A_{r(\lambda)} + \beta\, A_{b(\lambda)} + \upsilon\, A_{y(\lambda)}$$

where $A_{m(\lambda)}$, $A_{r(\lambda)}$, $A_{b(\lambda)}$, $A_{y(\lambda)}$ are the absorbance of mixture 3, red (12 dpl), blue (12 dpl), yellow (12 dpl) at λ and $\rho,\ \beta,\ \upsilon$ are the relative weights of $A_{r(\lambda)}$, $A_{b(\lambda)}$, $A_{y(\lambda)}$ respectively. $\rho,\ \beta, \upsilon$ was calculated using two methods: nonlinear regression and system of equations.

$\rho,\ \beta, \upsilon$ was calculated using least squares nonlinear regression by implementing the function curve_fit from the library SciPy (see Appendix A). The calculations resulted in ρ=0.4236, β=0.1429, and υ=0.4928. Using these coefficients, a model was created (Figure 3). A mean absolute error of 0.0140 was observed between mixture 3 and the nonlinear regression model.

Another way ρ, β, υ were calculated was by selecting three wavelengths and solving a system of equations. The three wavelengths that corresponded with the maximum absorption values from each solution were selected. This system was then solved:

$$A_{m(max\ blue\ \lambda)} = \rho A_{r(max\ blue\ \lambda)} + \beta A_{b(max\ blue\ \lambda)} + \upsilon A_{y(max\ blue\ \lambda)}$$

$$A_{m(max\ red\ \lambda)} = \rho A_{r(max\ red\ \lambda)} + \beta A_{b(max\ red\ \lambda)} + \upsilon A_{y(max\ red\ \lambda)}$$

$$A_{m(max\ yellow\ \lambda)} = \rho A_{r(max\ yellow\ \lambda)} + \beta A_{b(max\ yellow\ \lambda)} + \upsilon A_{y(max\ yellow\ \lambda)}$$

The calculations resulted in ρ=0.4177, β=0.1471, and υ=0.5005. Using these coefficients, another model was created (Figure 3). A mean absolute error of 0.0150 was observed between mixture 3 and the max value model.

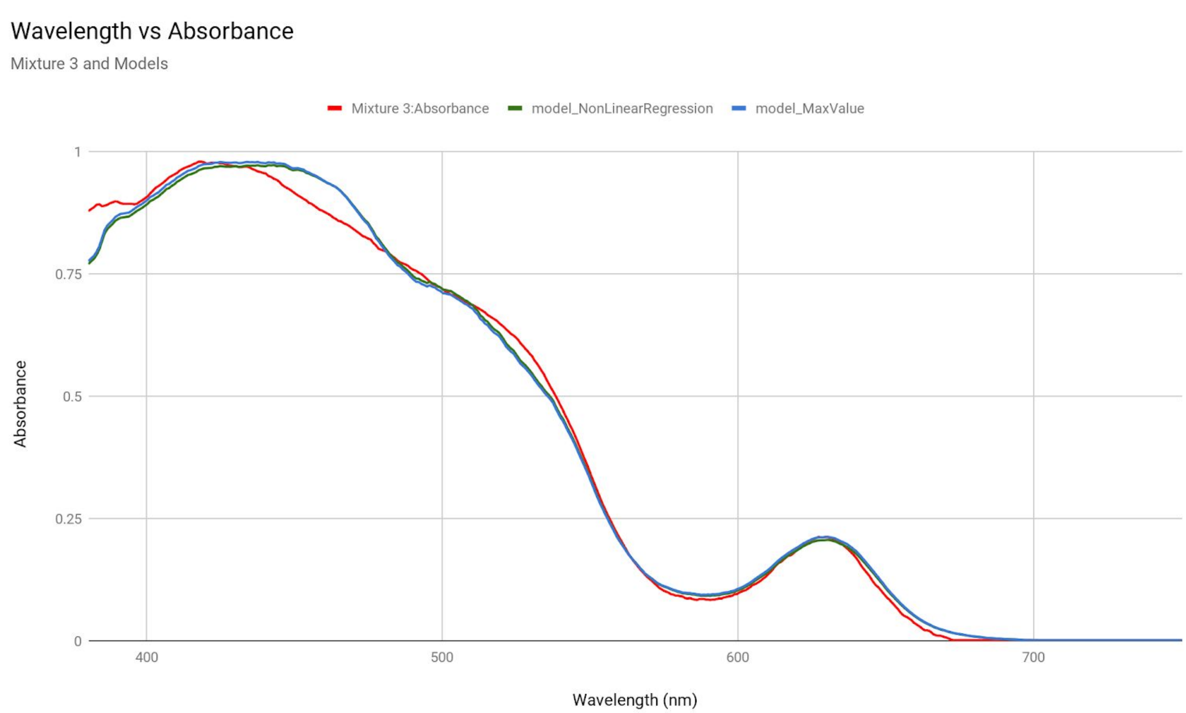

Figure 3 Relationship between wavelength and absorption of mixture 3 and models

While the nonlinear regression model and max value model were almost identical, the nonlinear regression model was deemed more accurate due to its lower mean absolute error value. To solve for the proportion of red, blue, and yellow solutions, ρ, β, υ from the nonlinear regression model was used. The proportions were calculated to be 5.084 dpl of red, 1.714 dpl of blue, and 5.913 dpl of yellow.

Conclusion:

Through this experiment, the concentration of dyes in an unknown mixture were predicted. This was done by quantitatively measuring the wavelengths and absorbances of solutions with known concentrations and an unknown mixture using spectrophotometry. Using this data, two models were constructed to determine the absorption of the unknown mixture. The accuracy of the two models was tested by calculating the mean absolute error. It was observed that the nonlinear regression model was slightly more accurate compared to the max values model.

The inaccuracy of model could be due to errors which could have happened during spectrophotometry. Errors such as imperfect calibration from our spectrophotometer and amount of liquid present inside and outside the cuvette could have affected our absorption values. However, these errors did not affect our model significantly based on the low mean absolute error.

Our experiment could be improved by using other various statistical algorithms such as the Levenberg–Marquardt algorithm to construct a model. In addition, using a similar procedure can seek to answer absorption differences in various brands of food coloring, to see which brand contains the most dye per drop.

References

Experiment 10.1 (n.d.). Retrieved January 13, 2019, from https://docs.google.com/document/d/1B-4HA3NZnfej2ifQVENSTrbXtt7TA_cz-3gYt2uGXTc

E., Oliphant, T., Peterson, P., & others (2001). SciPy: Open Source Scientific Tools for Python. Retrieved January 13, 2019, from http://www.scipy.org/

Meurer, A., Smith, C. P., Paprocki, M., Čertík, O., Kirpichev, S. B., Rocklin, M., . . . Scopatz, A. (2017). SymPy: Symbolic computing in Python. doi:10.7717/peerj-cs.103 Retrieved January 13, 2019, from https://www.sympy.org

Oliphant, T. E. (2015). A guide to NumPy. Austin, TX: Published by Continuum Press, a division of Continuum Analytics. Retrieved January 13, 2019, from http://www.numpy.org/

Vanderplas, J. T. (2017). Python data science handbook: Essential tools for working with data. Beijing: OReilly. Retrieved January 13, 2019, from https://pandas.pydata.org/

Appendix A

Source code is provided below.

https://colab.research.google.com/drive/1gB_fyO0sn9qpyck-g5BbxZZwsx69dlol

https://gist.github.com/hdko/7a2c8fe1d596a6089187c348eb607e76