

The Beer's Law Simulator

In the laboratory, you explored a variety of aspects of visible spectrophotometry in *More Lights, Color, Absorption*. You should have derived Beer's Law from experimental data. This simulation, using an interactive Excel spreadsheet, will enhance your understanding of Beer's Law and how a number of variables influence the absorbance being measured. The multi-sheet interactive Excel spreadsheet is on the CHM 103 webpage (<http://academic.pgcc.edu/~ssinex/chm103.html>). The tab, lower left, on the Excel workbook is used to move from sheet to sheet and is marked for each section below.

The Mathematics of Beer's Law - Concentration tab

Beer's law is a linear relationship between absorbance (A) and three independent variables: the molar absorptivity (a), the pathlength (b), and the concentration (c). The law takes the form of $y = mx + b$, where m is the slope and b is the y-intercept. So for Beer's law or $A = abc$, what is the value of the y-intercept?

For a plot of the absorbance as a function of concentration, what is the slope in terms of the independent variables?

In any Beer's law investigation, a certain wavelength is used and is held constant. What does the wavelength influence, since it does not appear in the mathematical statement of Beer's law?

Investigating the Calibration Curve (A vs. c) - Concentration tab

The linear calibration curve is one of the most powerful analytical tools for scientists.

How does changing the pathlength, b, influence the calibration curve? Sketch a graph.

How does changing the molar absorptivity, a, influence the calibration curve?

Why do the pathlength and the molar absorptivity have the effect you saw above?

The Effect of Pathlength (A vs. b) - Pathlength tab

The absorbance as a function of pathlength is another linear relationship.

What is the slope, in terms of any of the three independent variables, for this graph?

Investigating the Absorption Spectrum (A vs. λ) - Wavelength tab

The absorption spectrum is a plot of absorbance as a function of the wavelength. This is the first thing determined in any analysis, so that the wavelength of maximum absorbance, λ_{\max} , can be located on the plot. The remainder of the analysis is performed at this wavelength.

Looking at the absorption spectrum, where is λ_{\max} ?

If the concentration changes, does λ_{\max} change?

If the pathlength changes, does λ_{\max} change?

How does the absorption spectrum change when the pathlength is varied? when the concentration is varied? Sketch a graph.

What variable does the wavelength influence? (You might want to go back to the concentration tab)

How does this variation plot? Sketch it.

How does this relate to the absorption spectrum?

The Influence of Errors on the Calibration Curve - Concentration tab

The spectrophotometer was set-up and calibrated using a distilled water blank ($A = 0$). For the analysis, the blank used for the analysis contained other reagents and gave an absorbance of 0.15. How would this influence the calibration curve? If you did not notice the blank's actual absorbance, how would the graph point it out?

A student ran a calibration curve and then knocked the wavelength dial on the spectrophotometer, so that the wavelength increased by 20 nm. How are the subsequent results of sample analysis influenced? Explain.

Transmittance as a function of concentration (T vs. c) - Transmittance tab

Transmittance is simply the ratio of the outgoing light intensity divided by the initial light intensity or $T = I/I_0$.

What type of relationship is found for transmittance as a function of concentration?

If T drops in half (from 0.80 to 0.40), how does c change?

Absorbance ($A = -\log T$) was originally used to transform the data to a linear relation for ease of manual graphing. Today with graphing calculators and spreadsheets curve fitting is easy. Which relationship is easier to deal with – A vs. c or T vs. c? Why?

Extrapolating your calibration curve (A vs. c) - Bad Cal tab

What happens to calibration curves at high concentrations?

The bending downward at high concentrations is typical. The non-linear position of the calibration does not adhere to Beer's Law. Why?

How does this influence your final concentration if you were to extrapolate and use the linear calibration curve?

The educational value of this Excel simulation only comes from playing with it and trying to figure out what is going to happen. Then change the variable and see what happens. Learn and think about the situations posed NOT memorize! An answer key is available for this set of questions at: http://academic.pgcc.edu/~ssinex/BLS_key.pdf