Internet Connection

Online Chemistry Simulations to Intrigue, Engage and Attract 21st Century Science Students

by Linda Sawson

Undoubtedly the Covid-19 pandemic has revealed how little we have utilised computers and the internet for science teaching. Prior to the crisis, computers and the internet had been used by the majority for data spreadsheets, as word processors, and as a means of rapid communication.

As we look towards a post pandemic “new normal” it is right that we should address this issue by forging an ambitious and innovative marriage between the internet and science teaching. Simulators for Teaching Ltd., (Sim4t), formed in 2011 by a team of experts in scientific instrumentation and education has been at the forefront of innovation: We produce online software that simulates scientific instrumentation and experiments for chemistry and general science students in universities, colleges, and schools.

Enabling Educators

Sim4t has enabled educators to complement in-person teaching with simulations: for example, the School of Chemistry at University College Cork was looking for cost effective ways for advancing their laboratory classes but in a new and dynamic way, so simulation experiments were ideal. Similarly, the Department of Chemical Sciences at the University of Limerick, a user since 2018, had to design five undergraduate laboratory experiments as part of a new module. They have subsequently managed to advance how they teach and connect with over 30 additional chemistry students to their existing laboratory cohort, per semester, using Sim4t software, thereby improving teaching efficiency.

Significantly, this year, the opportunity to break the Covid-19 lockdown by providing online Sim4t experiments for students studying remotely has been seized upon by institutions in Romania, Italy, and the UK.

Flexibility

The key word in terms of how an institution may use Sim4t technology is *flexibility*:

- As a replacement for laboratory classes; classes can be expensive due to instrument and building costs, and staff time. Simulation offers a full online experiment for a fraction of the cost of a real laboratory.
- The software can be used as a pre-laboratory exercise to help students use their actual

laboratory time more efficiently or give them some “extra laboratory time” by using the simulator to follow up on things introduced in a formal laboratory class.

- The online system can be used for distance learning and by part-time students and thereby overcome logistical problems associated with delivering education to this group.
- The software can be used to promote self-study and independent learning amongst students and provide efficiencies in both staff time and how laboratory facilities are used.
- The choice is up to each individual institution.

So, what does the online portal offer?

Simulators for the Web (Sim4Web)

The Sim4t secure online portal, known as Simulators for the Web (Sim4Web), is based on a UV-Visible Absorption spectrometer simulator. Currently, we offer seven experiments covering topics from an “Introduction to UV-Visible Absorption Spectroscopy” through “Qualitative and Quantitative Analyses” and onto “Chemical Kinetics.” Users must register to access the Sim4Web secure platform via an e-mail address and password. There are two types of user defined by the system: supervisor and student, respectively.

Sim4Web allocates different privileges and access to documentation depending on the user status. As a supervisor, one can create an experimental session and invite students onto that session. A supervisor can also run an experiment for themselves: A typical Home Screen is shown in Figure 1. Navigation through the software is achieved via the menu list on the left-hand side of the screen working down through from top to bottom allowing access to the virtual materials, glassware and instrumentation necessary to perform repeated runs of an experiment.

Documents

Documentation for each experiment is accessed via the “Documents” submenu shown in Figure 1. This includes a complete experimental procedure which guides the user through operation of the simulator and the experiment, detailed lecture notes covering the theory of the topic and model answers (for supervisors only).

Qualitative and Quantitative Analyses

Experiment 1 in the Sim4Web catalogue is “The Beer-Lambert Law and Identification of an Unknown Mixture” and introduces the concepts of *qualitative* and *quantitative* analyses.

The first part of this exercise, involves preparing virtual samples and recording UV-Visible spectra for naphthene, anthracene, and perylene, respectively, in toluene solution. Beer-Lambert plots are then constructed for each aromatic species and the molar absorption coefficient (ϵ), determined. In the second part of the experiment, unknown samples, allocated by the supervisor to each individual student, are investigated. Given the information derived in part one, UV-Visible spectroscopy will be used qualitatively to identify the species, and then quantitatively to determine the amount of each component present in the unknown sample.

The Virtual Flask

The virtual flask module (shown in Figure 2, for perylene) allows repeated attempts at sample preparation of a stock solution from the “Create Stock Solution” menu. The desired flask size is selected via a drop-down menu and virtual chemicals can be weighed out and solvent added up to the graduated mark via the slider control under the flask. Similar modules allow dilutions of a stock solution to be created via the “Create Dilutions” submenu.

The Spectrometer Simulator

Once the virtual samples have been prepared, they can be run on the spectrometer simulator accessed via the “Measure Spectra” submenu. The spectrometer set up screen is shown in Figure 3a). This menu allows selection of the measurement mode: either a full scan or single wavelength readout. In the full scan mode, the wavelength range can be defined in addition to the scan speed.

A solvent reference must be run prior to each spectroscopic sample measurement. The spectrometer scan window for an unknown mixture is shown in Figure 3b). Data can be displayed in either Absorbance or Transmittance mode with a cursor available to generate point intensity readings at a given wavelength.

Figure 1. The Home Screen

Figure 2. The Virtual Flask

Figure 3. The Spectrometer Simulator

Learning Outcomes

The experiment provides practice in sample preparation and solution dilutions in addition to operation of the spectrometer simulator.

Chemical Reaction Kinetics

Two experiments covering chemical kinetics are currently offered via the Sim4Web platform, both based on the reaction of crystal violet (CV) with sodium hydroxide (NaOH). One experiment allows the empirical determination of the rate law (described

Figure 4. The Wet Bench

in the following section) while the second concerns the temperature dependence of the reaction and Arrhenius behaviour.

CV is an intensely coloured triarylmethane dye, that transforms into a colourless product on reaction with NaOH. Consequently, the absorbance of a reaction mixture containing CV and NaOH will be proportional to the concentration of unreacted dye still present in solution. The reaction of CV and NaOH can therefore be monitored and the kinetics studied by measuring the absorbance of the mixture as a function of time. By using the Beer-Lambert law, if ϵ for CV is known, the concentration of CV can subsequently be derived as a function of time.

The rate of the reaction or rate law between CV and NaOH can be written:

$$\text{Rate} = k [\text{OH}^-]^x [\text{CV}]^y \quad (\text{eq. 1})$$

where k is the rate constant (or rate coefficient) for the reaction, x is the order with respect to OH^- and y is the order with respect to CV. In this experiment, students are tasked with determining, experimentally, the value of x and y . In order to do this, the reaction (and the kinetics) is simplified by using a vast excess of NaOH: it can therefore be assumed, that the concentration of hydroxide ion does not change through the course of the reaction even though all of the CV may have been used up. Consequently, the $[\text{OH}^-]$ term in the general rate law is constant and can be grouped with k as in equation 2:

$$\text{Rate} = \{k [\text{OH}^-]^x\} [\text{CV}]^y \quad (\text{eq. 2})$$

where $k' = k [\text{OH}^-]^x$ (k' is termed a *pseudo* rate constant or the *observed* rate constant.)

The rate equation can, therefore, be written:

$$\text{Rate} = k' [\text{CV}]^y \quad (\text{eq. 3})$$

This approximation simplifies the reaction and allows k' and y to be determined experimentally by carrying out two reactions: in the first kinetic run the concentration of NaOH is half that used in the second experiment. For both reactions, the $[\text{OH}^-]$ is vastly in excess of that of CV.

Once k' has been derived it is possible to determine k and x since the concentration of NaOH is known in both experiments.

This experiment is composed of 2 parts: initially students must make up a stock solution of CV and then prepare a series of dilutions to allow ϵ to be determined.

The second part of the experiment is concerned with using an absorption spectrometer simulator to monitor the kinetics of the reaction by using a virtual wet bench as shown in Figure 4.

By clicking "add CV to beaker" a virtual pipette releases 9 cm^3 of a $10^{-5} \text{ mol dm}^{-3}$ CV dye solution into a beaker (see Figure 4a). The desired wavelength (λ) of interest can then be selected by clicking "Set Wavelength." (This should be the same λ that was used to derive ϵ in Part A of the experiment).

The reaction is initiated by clicking "add NaOH to beaker" wherein a virtual pipette releases 1 cm^3 of a 0.05 mol dm^{-3} NaOH solution into the beaker containing the CV dye. (The effective concentration of NaOH in the reaction is, therefore, $0.005 \text{ mol dm}^{-3}$.) The clock must be started immediately the transfer has been made. A sample of the reaction mixture is extracted via a virtual pipette and transferred to a cuvette.

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By clicking the “Start Spectrometer” button, the sample is loaded into the spectrometer (as in Figure 4b) and an absorbance reading taken as soon as possible, noting the time of the measurement. The absorbance readings should then be converted into concentrations using the Beer-Lambert law and the value of ϵ for CV in aqueous solution determined in Part A. (Enough 0.05 mol dm⁻³ NaOH solution has been allocated by the software to perform a further two kinetic runs if desired).

The software allows a second kinetic experiment to be run following the same procedure as outlined above but using a 0.1 mol dm⁻³ NaOH solution.

Data Treatment

The students must first work out the concentration profile of CV during the course of the reaction using the ϵ value determined in Part A. The data should subsequently be plotted to determine whether the reaction is zero, first or second order.

Learning Outcomes

The experiment provides practice in sample preparation and solution dilutions in addition to operation of the spectrometer simulator. The kinetics segment of the experiment offers experience in quick and careful addition of a reactant to start a reaction while carefully coordinating the start of the stopwatch and extraction of a sample for analysis. Practice in careful monitoring and recording of the absorbance as a function of time forms the latter practical aspects of the experiment.

How to treat data and plot graphs correctly to derive meaningful physical constants from the gradient is also a learning outcome from this experiment.

What do Students Think?

Perhaps it is appropriate at this point, to leave the final word to the students themselves:

A recent survey, commissioned by Sim4t, revealed that over 97% of student respondents liked the accompanying documentation (*i.e.*, lecture notes, experimental procedures, and user manuals) and found it extremely helpful.

Furthermore, 95% of the pool said that the combination of the virtual flask module and the spectrometer simulator was very useful for their studies and that they would like to have online chemistry simulations to complement their current science programme.

In Summary

Sim4t provides a cost effective, fully interactive, online learning system (Sim4Web) which will allow institutions to provide innovative and engaging material, effectively deliver distance learning, widen access to science education for all and improve teaching efficiency in the 21st century educational market.

For more information about the simulations and products that Sim4t offer please go to the company website: www.sim4t.com
visit the Sim4t YouTube channel:
<https://www.youtube.com/channel/UCezS564e-gpKuvqJEQjJRAg>
or e-mail: l.swanson@sim4t.com