

Chapter 17

CUSTOM DEVELOPED SOFTWARE TO SIMULATE THE USE OF UV/VIS SPECTROSCOPY IN QUANTITATIVE CHEMICAL ANALYSIS

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ABSTRACT

Software which simulates the use of typical analytical chemical techniques provides students with additional ways of learning about these techniques. This chapter presents a free software package called UV-Vis-Sim, which can be used to simulate the use of an Ultraviolet/Visible (UV/Vis) spectrometer in quantitative chemical analysis. UV/Vis spectroscopy uses a simple linear model of absorbance, the Beer-Lambert Law. For quantitative information on a compound, the UV/Vis instrument must first be calibrated using solutions of known concentrations: the calibration curve generated allows measurement of unknown concentrations of that compound. The software allows any compound to be analysed if its UV/Vis spectrum is known. The instructor version can be used to define constraints similar to those encountered in the lab. Students use the student version to “prepare” their set of standard solutions based on their own calculations. The program then measures the absorbance of standards and unknown sample(s). The results can be copied into a spreadsheet and the data treated following standard procedures. The data will be individual to the students, depending on their choices and calculations. The software was used in a problem-based learning exercise, to simulate the analysis of samples from a potentially contaminated river.

Keywords: spectroscopy, chemistry, simulation software, problem-based learning.

1. INTRODUCTION

There is a strong drive to enhance student employability by developing students’ transferable skills, including critical thinking, problem solving, team working, and communication skills. The aim is to make graduates more employable, and increase their chances of succeeding in their future careers, which will benefit the graduates themselves, as well as the economy and society as a whole (Pegg, Waldock, Hendy-Isaac, & Lawton, 2012). Problem-based learning (PBL) has been successfully used to enhance students’ employability skills: students learn about problems or real life scenarios in a relevant context, they encounter a problem and are encouraged to explore potential solutions which, in turn, encourages them to develop their autonomy and take responsibility for their own learning (Martin, West, & Bill, 2008). PBL has been successfully used across a wide range of science subjects, including chemistry (Belt, Evans, McCreedy, Overton, & Summerfield, 2002; Belt, Leisvik, Hyde, & Overton, 2005), physics and astrophysics (Institute of Physics, 2014; Raine & Symons, 2005), and medical sciences (Wood, 2003).

A problem-based approach can increase students’ motivation, encourage independent learning, and create effective problem solvers with a broad range of interpersonal and professional skills (Belt et al., 2002). Although typically there is no significant difference in academic achievement between PBL and traditional students, research indicates that

students develop an improved attitude towards learning when PBL is used. For example, White and colleagues (2004) compared two groups of family doctors enrolled in a Continuing Professional Development course, one using small-group PBL and one a didactic lecture approach, in terms of the effectiveness and student satisfaction. There was no significant difference between the groups with respect to knowledge acquired, but the PBL participants rated the educational value of the program higher than the participants enrolled in the lecture course.

Spronken-Smith (2005) reported that geography students enrolled in a research methods course valued the benefits of a PBL approach. The students commented positively on the opportunity to enhance their teamwork skills, valuing the possibility of working in groups on authentic problems that they saw as relevant to their future careers. The students mentioned increased workload as a difficult aspect of PBL, and they felt more time was needed to engage with the PBL scenario in a meaningful way. Duncan and Al-Nakeeb (2006) studied the impact of PBL on students' learning experience in a third year Sports Science module. The researchers concluded that the use of a PBL approach appears to offer advantages in terms of student enjoyment, engagement and development of criticality compared to traditional lecture-led delivery. Students also seemed to perceive that they had a greater ownership of their own learning when following a PBL curriculum. As in the previous case, workload was identified as a potential barrier for PBL, and the researchers highlighted that an appropriate amount of time is needed to allow students to engage with the PBL scenarios effectively.

While technology is not a required component of PBL, it can play an important role in the PBL process, improving the flexibility and quality of the learning and enhancing the student experience (Park & Ertmer, 2008). Most graduates will find themselves in workplaces where technology is embraced as an essential tool, and technology-enhanced PBL can provide a context in which technology skills are developed alongside problem solving skills. Technology can enhance the authenticity and relevance of the PBL scenario (Park & Ertmer, 2008). It can be used as a tool to collect relevant data or recent information about the problem. Students can use technology similar to that used in the workplace to organise and analyse the data and present solutions. Finally, students can use technology (e.g. presentation or video software) to present their findings.

One aspect of the use of technology in PBL is the use of custom-developed software to recreate the immediacy and complexity of the workplace, where decisions are frequently based on incomplete evidence. Software can be used to develop interactive scenarios, in which the data generated and the information available depend on the students' decisions. The authors of this chapter have created JPollution, custom made software capable of simulating environmental surveys; the software allows instructors to create pollution maps, set the number of samples that can be taken, and whether these will be visible immediately or the sample run must be completed before all the results are shown (Bertolo & Clay, 2006).

A team of researchers based at the University of Queensland has developed a suite of software tools (Scenario Based Learning - interactive, SBLi) to enable lecturers to easily develop interactive multimedia scenario-based lessons, which can be delivered to learners via CD, DVD or online (Norton et al., 2012). SBLi consists of a suite of software tools: the SBLi Builder, Player and Server, and is based on an earlier, pre-web computer-based learning tool. Breakey, Lenvin, Miller, and Hentges (2008) have used SBLi to develop a virtual genetics laboratory: the resource simulates the steps of a genetics experiment, and can be used to complement theory sessions in a genetics module. Seddon, McDonald, & Schmidt (2012) investigated the performance of student cohorts from a second-year

genetics course for undergraduate veterinary students, where SBLi was used to construct eight new PBL scenarios. Students appreciated the use of authentic scenarios, and comparison of learning outcomes from PBL and non-PBL-supported topics (within and across student cohorts) indicated that exposure to PBL generated quantifiable improvements in learning in both high and low ability students. The researchers concluded that SBLi software had the potential to improve the student learning experience, but noted that it was crucial to consider students' perceptions of scenario relevance, their confidence, and how students of differing learning styles engage with such computer-mediated activities.

As part of our ongoing interest in the development of free software which can be used to enhance PBL exercises, herein we present a software package called UV-Vis-Sim, which can be used to simulate the use of an Ultraviolet/Visible (UV/Vis) spectrometer in quantitative chemical analysis. The software comprises two programs, UV-Vis-Sim, used by the students to generate the data, and UV-Vis-Sim-Pro, used by the lecturer to generate the parameters under which the students will perform the virtual experiment. This software can be used to complement UV/Vis spectroscopy experiments, by providing students with additional opportunities to generate data, and then using this information to draw conclusions and extract quantitative information. The program is currently being trialed in a PBL scenario with first year Environmental Science students.

2. THE SOFTWARE

UV/Vis spectroscopy is an analytical technique which uses a simple linear model of absorbance, the Beer-Lambert Law. In order to obtain quantitative information on the concentration of a given compound, the UV/Vis spectrometer must first be calibrated using solutions of known concentrations. Once this so-called calibration curve is generated, unknown concentrations of the chemical can be measured (Clark, 2007). The technique, often used in the chemistry undergraduate laboratory, has a wide range of applications in real life, such as the quantitative determination of solutions of transition metal ions, some organic compounds and biological macromolecules.

UV-Vis-Sim is a free software package which can be used to simulate the use of an UV/Vis spectrometer in quantitative chemical analysis. The software is released under the GNU General Public Licence, GPL (2007). The GPL allows unrestricted copying, distribution and modification of the program, subject only to the requirement that the source code, and any modification, is made available to anyone who wishes to receive it. Both the source code and the compiled forms of the software can be obtained from the authors.

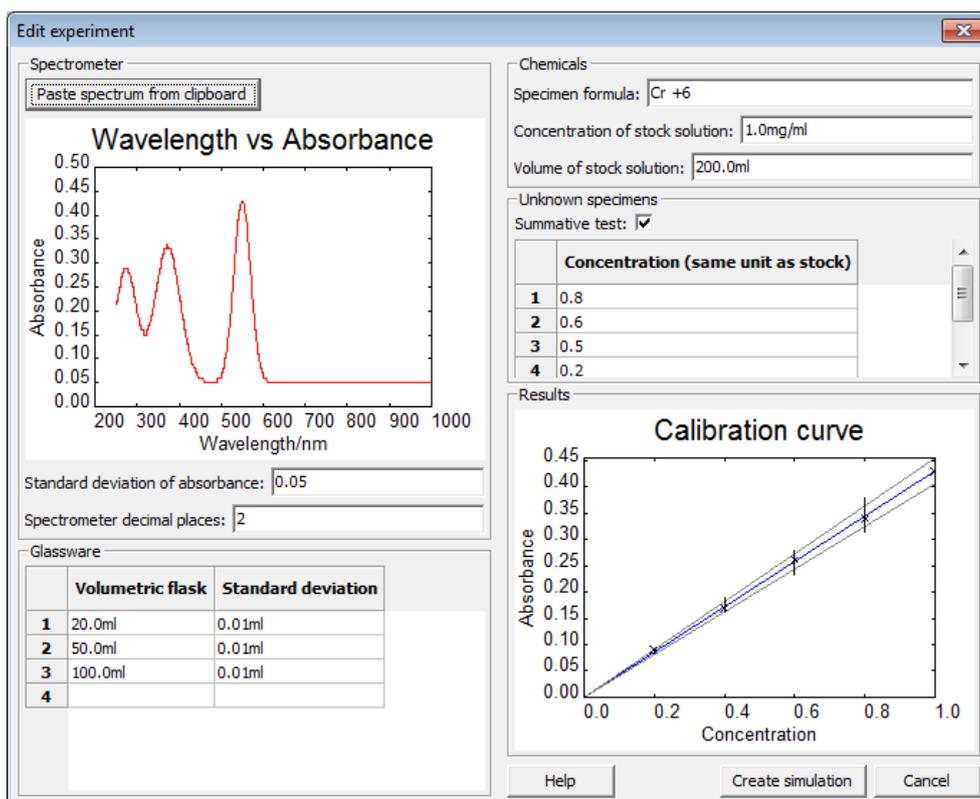
The software comprises two programs, UV-Vis-Sim (the student version) and UV-Vis-Sim-pro (the instructor version). Figure 1 shows a screenshot of the “create new experiment” dialog of the instructor version. In this dialog it is possible to define constraints similar to the ones students would find in the lab, including the spectrum, available glassware, the volume and concentration of the stock solution, and the concentrations of the unknown samples. Random errors can be added at various stages, to simulate real experimental errors. Any compound can be analysed, as long as the UV/Vis spectrum of that compound is known.

Two types of experiments can be created, depending on whether or not the “summative test” tick box is selected. If it is selected, the instructor can define one or more “unknown” samples and set the concentration for each of them. The students will not see the concentrations, so this mode is useful to set up PBL scenarios. If the “summative test”

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option is not selected, the program will generate a random unknown sample each time the student loads the experiment. It will also provide the opportunity for the student to enter their estimate of the concentration and check whether or not it is correct. This mode could be useful to complement a lab session by providing additional practice outside the lab.

Figure 1. Screenshot of the “Create new experiment” dialog in the instructor version. The example will simulate an experiment with four “unknown” samples of Chromium VI.



Once the simulation is set up, it can be saved as a file and opened in the student version. Students can “prepare” their own set of standard solutions, choosing the number of solutions and their concentrations for themselves (limited by the amount of stock solution and the glassware available). Students specify both the concentrations that they desire, and the volume of stock solution to be used. The program disregards the concentration values, and uses the volumes to calculate the “real” concentration and calculates the absorbance based on that value. The program then displays the absorbances of the standards and the unknown sample(s). The results, which show the students' desired concentrations rather than the “real” ones, are presented in tabulated form which can be copied into a spreadsheet and the data treated following standard procedures. The data will be individual to the students, depending on their choices and calculations. Figure 2 shows a screenshot of a set of results generated with the student version.

Figure 2. Screenshot of a set of results generated with the student version, using as basis the experiment for Chromium VI set up on Figure 1. The values for absorbance are generated after the student clicks “run experiment”. The “copy results” button copies the data into Clipboard. This experiment is in summative mode; in formative mode, the “Unknown concentration” box would be active and students could check that their concentration estimates are correct.

UV-Visible Spectrometer Simulation

File Help

Spectrometer settings
Wavelength/nm: 549.2 Select wavelength...

Stock solution
Concentration: 1.0mg/ml
Volume: 200.0ml Remaining volume: 80.0ml

Experiment

	Concentration (mg/ml)	Volumetric flask	Stock volume	Absorbance
1	Unknown sample 1:			0.34
2	Unknown sample 2:			0.24
3	Unknown sample 3:			0.21
4	Unknown sample 4:			0.09
5	0	100.0ml	0	0.0
6	0.2	50.0ml	10	0.09
7	0.4	50.0ml	20	0.16
8	0.6	50.0ml	30	0.26
9	0.8	50.0ml	40	0.33
10	1.0	50.0ml	20	0.16
11				

Run experiment

Results
Copy results Unknown concentration: Check...

3. THE PBL EXERCISE

A PBL scenario has been developed based on this software, to simulate the study of samples from a potentially contaminated river. The scenario was inspired by a similar one called “Tales of the Riverbank”, developed by Belt, Overton, and Summerfield (2002). It was trialed with approximately 90 first year undergraduate Science students, running over the course of 4 weeks. Students worked in groups and were asked to act as environmental consultants for the Unitown River Authority. The authority had received a complaint about a perceived reduction in number and size of fish caught along the River Dribble, which runs

through the town. Their task was to identify whether there was a pollution issue, and suggest further action if needed. Students presented their findings as a written group report, although other modes of assessments, e.g. individual/group presentations could also be used. Students were given a map of the area, which showed the fishing sites affected and various potential sources of pollution (arable land, an electroplating company, water treatment plant, etc.). They were also provided with summary of businesses discharging into the River Dribble, and typical composition of their discharge effluents.

In the initial session students brainstormed what additional information/data they needed, and how that could be obtained. Over the following weeks, students were provided with UV-Vis-Sim files which contained the necessary information to generate data for Chromium VI and Chlorite levels respectively from 10 sampling sites. Additional data to inform their report were fish size data for the two fishing sites at the river Dribble, and a discharge water quality report from the Unitown Water Treatment Plant, containing a selection of physicochemical (e.g. pH, temperature), biological (E.coli) and chemical (organic compounds, anions and metal ions) parameters.

Informal feedback from students was very positive. Students reported no problems with the software, and they found the possibility of generating their own set of data to be stimulating. A common request was the possibility of generating more data themselves, instead of using already prepared data. This has been taken on board, and in future years students will be able to generate data for other chemical parameters besides Chromium VI and Chlorite. Future work will also include the full evaluation of the student experience.

4. CONCLUSION AND FURTHER WORK

This chapter presents a free software package, developed by the authors, called UV-Vis-Sim, which can be used to simulate the use of a UV/Vis spectrometer in quantitative chemical analysis. UV-Vis-Sim can be used to complement UV/Vis spectroscopy experiments, by providing students with additional opportunities to generate data, and then using this information to draw conclusions and extract quantitative information. The software has been used in a PBL scenario with first year undergraduate Science students, to simulate the study of samples from a potentially contaminated river. Informal feedback from students has been very positive. Students appreciated the highly interactive aspect of this part of the scenario, and suggested that future cohorts could generate their own data for other parameters using the software.

Future work will include the revision of the PBL scenario in light of the comments received by this first group of students, and a full evaluation of the student experience. With regards to the program itself, assessing the impact of the program on the student learning experience is a challenging task. UV-Vis-Sim is just another tool to enhance a PBL scenario and, like all tools, it can be used effectively or poorly by those who design the scenarios. Whether the learner's experience is enhanced or not will depend on the full PBL scenario, and how well this scenario has been integrated into a particular lesson or module.

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