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Technology Report

Simple Visual-Aided Automated Titration Using the Python Programming Language

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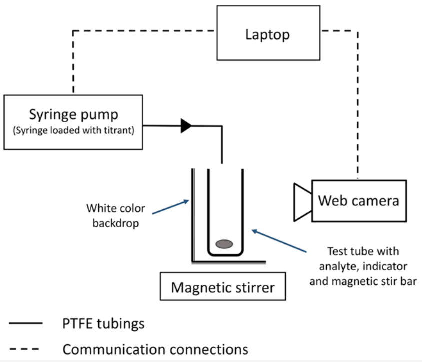
ABSTRACT: The advance of digital technology presents an opportunity to equip students with relevant skill sets as "Scientists of the Future" who are able to utilize knowledge at the interface between various disciplines. In this technology report, an open source programming language is used to automate a simple laboratory experiment commonly performed by Chemistry and Chemical Engineering students. It is introduced and demonstrated to the students from a 3-year Chemical Engineering undergraduate program. The aim of this activity is to allow students to appreciate the integration of knowledge from Chemistry and Computer Science.



KEYWORDS: *Second-Year Undergraduate, Upper-Division Undergraduate, Analytical Chemistry, Interdisciplinary, Laboratory Equipment, Computer-Based Learning, Acids/Bases*

■ INTRODUCTION

Automated equipment is an integral part of a modern laboratory in the chemical industry. Automation has alleviated tedious and repetitive work such as weighing and dispensing liquids, allowing scientists to focus on more creative activities.[1] Furthermore, automation has been argued to lower the hurdles to access new techniques, thereby fostering chemistry innovation.[2] Automation in chemical analysis was available as early as 1914[3] and has since been widely applied to chemical synthesis.[4,5a−d] The use of computer-based technology for automation in academic chemistry research laboratories[6] and in the area of artificial intelligence and machine-learning[7,8] has received particular attention in recent years.

Technology disruption in the chemical industry is a continual process, and it would be beneficial to consider how the next generation of chemists and chemical engineers could receive foundational training in these technologies, allowing them to be competitive in the job market.[9−11] The use of computer-based technology to complement a Chemistry experiment common to students is explored as a consideration of the skills required by a "Scientist of the Future".

The simple visual-aided automated titrator described herein demonstrates the application of such a technology in a common laboratory experiment. This concept is inspired by works published by Ley and co-workers[12] and Mellado-Romero and co-wokers.[13] The automated titration setups previously reported typically used potentiometric changes for feedback.[14a−f]

As argued by Bell,[15] the students' understanding of instrument theory and computer skills may vary across a cohort or between different disciplines such as Chemistry and Chemical Engineering. The incorporation of automated instrumentation is by no means a substitute for knowledge and hands-on laboratory technique but yet could illustrate improvements in efficiency. The assembly of a simple automated setup would enhance the students' confidence with knowledge required to match the pace of technology advancement. Students could gain Computer Science knowledge through a dedicated course in collaboration with their tertiary institution's Computer Science Department.[16] Alternatively, relevant concepts could be introduced progressively through existing chemistry courses by revision of traditional experiments to include concepts in automation.

The setup described in this technological report aims to provide laboratory instructors with a resource to allow undergraduates to take an interdisciplinary approach for a common chemistry experiment. An open-source programming language (Python)[17] is used with equipment found in a Chemistry laboratory. It is envisioned that students would come to appreciate the interdisciplinary nature of science and also learn how technology could automate routine tasks. A

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short survey was conducted with a small group of student and teaching staff to gather feedback on this setup.

AUTOMATED TITRATOR SETUP

An automated acid−base titration of aqueous hydrochloric acid with aqueous potassium hydroxide, using a phenolphthalein indicator, was chosen for this setup. The main equipment required are a laptop, programmable syringe pump, and a web camera. A full list of equipment and parts is available in the Supporting Information.

The setup is described schematically in Figure 1. The syringe pump and web camera are both connected to the laptop via a USB connection. The syringe mounted on the pump has a PTFE tube leading to the top of the test tube. A photograph of the setup is shown in Figure 2.

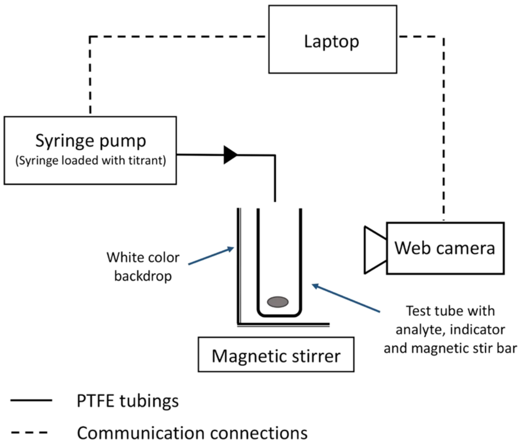

Figure 1. Schematic diagram of the visual-aided automated titration system. The laptop computer communicates individually with the syringe pump and web camera using USB cables.

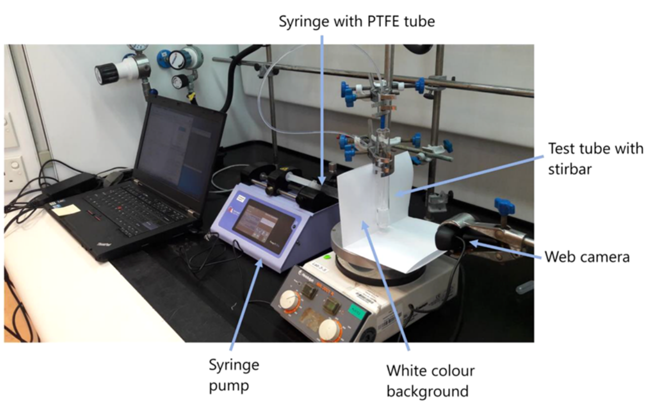

Figure 2. Photo of the experimental setup. A piece of white paper is used to provide the white background for the color detection through the web camera.

A 10 mL disposable plastic syringe is filled with aqueous 0.1 M potassium hydroxide solution, fitted with the PTFE tubing, and the tubing primed before being secured on the syringe pump. A 4.0 mL volume of 0.1 M aqueous hydrochloric acid analyte was added to the test tube positioned, as shown in Figure 2, using a calibrated glass pipette or a single channel pipette. A drop of phenolphthalein indicator was then added. A PTFE stir bar and magnetic stirrer were used to mix the solution in the test tube during the titration.

The Python code used for automation utilizes two additional packages. “Pyserial” enables the computer to communicate with devices connected via USB,[18] whereas “Pyautogui” enables the computer to determine the RGB color of a given pixel on the computer screen.[19] Addition of aqueous potassium hydroxide titrant from the syringe pump was initiated by the Python code. As the titrant is being added, the USB web camera displays a view of the test tube on the computer screen. The syringe pump would be automatically stopped once the end point pink RGB values are detected at the designated pixel positions on the screen. For this reason, the phenolphthalein indicator has the advantage of a distinct color change from colorless to pink when the titration end point is reached, allowing for a sensitive response from the code. Calibration of the end point RGB color is documented in the Supporting Information.

The volume of titrant dispensed by the syringe pump could be obtained at the end of each experiment, as shown in Figure 3.

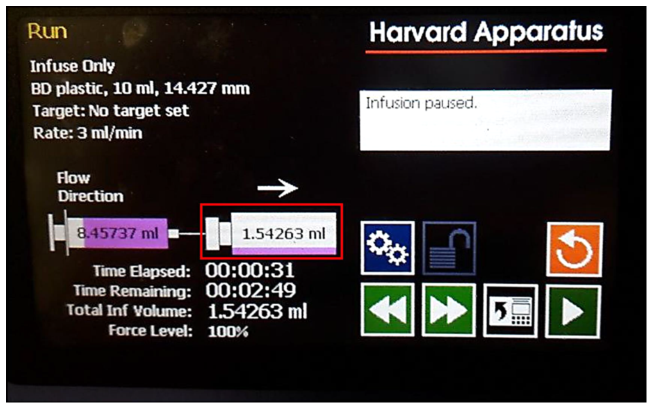

Figure 3. Example of the touch-screen display on the syringe pump showing the volume of titrant dispensed (red box).

Calibration of the pump was conducted at three different flow rates, with the results shown in Table 1. The displayed volume of titrant dispensed was typically greater than the actual volume dispensed. Full data are described in Appendix 1 of the Supporting Information.

Table 1. Calibration of Pump Flow Rates

Flow Rate, mL/min	Average Percentage Error[a]	Standard Deviation of Percentage Error
0.80	−0.76	0.06
2.00	−0.60	0.08
3.50	−0.69	0.20

[a]The average % error is with respect to the value displayed by the pump.

HAZARDS

The phenolphthalein indicator (0.25 wt % in 1:1 ethanol/water) is flammable, an irritant, and classified as a potential carcinogen. Potassium hydroxide (0.1 M) and hydrochloric acid (0.1 M) are corrosive. All personnel are required to wear a lab coat, safety goggles, and nitrile gloves to prevent direct skin

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J. Chem. Educ. 2020, 97, 850−854

and eye contact. All chemical handling and operations should be performed in a well-ventilated fumehood.

■ RESULTS AND DISCUSSION

The setup requires a compatible laptop, web camera, and a programmable syringe pump that can be controlled via serial commands. Other combinations of acid−base with their respective indicators of choice could be used, as their corresponding end point color (that is their RGB color values) could be amended in the Python code.

Use of Automated Titrator to Complement Existing Curriculum

From a chemical education point of view, the demonstrated setup provides an excellent opportunity for students to adopt a hands-on approach with the assembly. The knowledge gained from setting up the tube fittings could be extended to assembling a flow reactor involving similar tubes and fittings.

The code uses common principles in Computer Science (e.g., declaration and assignment of a variable, looping structure, control structure, printing output, threading) and could be segmented into different sections whose size is dependent on the students' proficiency level with the Python programming language. The task of the students would be to rearrange these sections, like a jig-saw puzzle, in the correct sequence for the code to run in the desired manner, hence facilitating the learning outcome of gaining basic coding knowledge (see Supporting Information).

In a traditional acid−base titration experiment, the volumes of titrant and analyte used are typically determined by the error associated with obtaining an accurate volume reading from a graduated burette containing the titrant. The repeated actions of manually adding the titrant, swirling the flask, and observing a color change are easily implemented by a code with better reproducibility. The automated setup thus served to augment the existing manual acid−base titration experiments, with the students providing critique to both methods.

In this Python code, the end point was defined as the two chosen pixel coordinates having the same pink RGB values. It was observed that nearing the end point of the titration, the pink coloration tends to persist briefly before it disappears as the solution is being mixed. Thus, receiving feedback from the color at two pixel coordinates reduces the chance of a false end point. Conversely, a single-pixel coordinate may be used intentionally to obtain a false end point. Students could perform data analysis from repeated experiments to determine the deviation from the actual end point by comparing it with existing manual titration experiments. This would encourage students to think critically and suggest improvements to the current setup or Python code.

The use of a syringe pump, with the volume of titrant dispensed shown, provided students with the opportunity to discuss the experimental errors involved with this setup and critique the precision and accuracy of this method. The average volumes of titrant used to neutralize the acid from the manual setup and the automated titrator are shown in Table 2. Given the error associated with the graduated burette used, a larger volume of 15.0 mL of analyte was titrated using the manual setup, presumably providing the more accurate result. The average titrant volume of 15.19 mL was normalized to 4.05 mL for comparison with the case whereby a 4.0 mL equivalent of analyte would be used. The difference between the volumes of titrant used for the manual setup and the automated titrator is approximately between 2 and 5%.

Table 2. Comparative KOH Titrant Average Volume Experimental Results

Titration Method		Average Amount of 0.1 M KOH, mL	Standard Deviation
Manual[a]	Average	15.19	-
	Normalized[c]	4.05	0.02
Automated[b]	Flow Rate, mL/min		
	0.80	4.17[d]	0.03
	2.00	4.14[d]	0.03
	3.50	4.26[d]	0.02

[a]Five replicate experiments of 15.0 mL of 0.1 M HCl using a manual setup. [b]Five replicate experiments of 4.0 mL of 0.1 M HCl using the automated titrator at three different flow rates. [c]Normalized to a 4.0 mL equivalent of HCl analyte for comparison with the automated titrator results. [d]Corrected volume based on calibrated flow rates, not the volume displayed on the syringe pump.

Based on the results obtained for the automated titrator at different flow rates, a high flow rate of 3.50 mL/min gave a larger average volume. The most likely cause for this deviation could be a pause of 0.5 s in the code before the next iteration to obtain the RGB values. The volume dispensed during this pause duration becomes significant at higher flow rates. Interestingly, a low flow rate of 0.8 mL/min arguably did not result in better performance when compared to a flow rate of 2.0 mL/min. At low flow rates, the titrant would accumulate as a droplet at the tip of the PTFE tubing. This happened while the displayed dispensed volume continually increased, before the droplet eventually dripped into the test tube. Full data are shown in Appendices 2 and 3 of the Supporting Information.

Demonstration of Automated Titrator and Evaluation by Students

This learning activity was introduced to a group of 12 third year Chemical Engineering undergraduates and teaching staff during their visit to the Institute of Chemical and Engineering Sciences. This demonstration has components that allow teaching, development, and deployment of control algorithms.

A short introduction to the Python programming language as part of any course would be beneficial to the students' understanding of this activity. The feedback from students on this activity and topic is summarized in Table 3.

The survey results suggested that the participants were mostly positive to the learning outcomes of this demonstration, albeit with a small sample size. The survey served as a platform to understand user experience for this activity and would be extended to a wider audience once resources are available.

The aim of using an enabling technology in this automated titration experiment is to give students insights to the application of programming language to support teaching and learning at the university level. Students should be able to recall their experiences in a chemistry laboratory and also appreciate the use of programming activities to automate a task, thus connecting and applying knowledge across disciplines for problem solving. According to the survey, students found the setup closely related to the concepts learned in class and were keen to know more about the potential of using Python programming language.

This learning activity would be useful for Chemical Engineering undergraduates, helping them recall learning

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J. Chem. Educ. 2020, 97, 850−854

Table 3. Survey Response from a Group of Chemical Engineering Undergraduates and Teaching Staff

	Survey Questions	Students' Responses by Score, N					Score, Average (N = 12)	Standard Deviation
		1	2	3	4	5		
1[a]	Do you think the automated titration setup has illustrated concepts learned in class?	0	0	5	5	2	3.75	0.75
2[a]	Do you think open-source programming languages (e.g., Python) have advantages as compared to commercial scientific programming languages (e.g., MATLAB)?	0	0	2	7	3	4.08	0.67
3[b]	Considering that Python does not have a drag-and-drop graphic user interface (GUI)/simulator, how easy do you think it is to learn Python?	1	3	3	4	1	3.08	1.16
4[c]	Considering that Python does not have a drag-and-drop graphic user interface (GUI)/simulator, how willing are you to choose Python over a GUI-based simulator?	0	2	4	5	1	3.42	0.90
5[d]	How keen are you to find out other potential applications, or mini projects, using the Python programming language on your own?	0	1	4	4	3	3.75	0.97

[a]Scale range for Q1 and 2: 1, Strongly disagree; 3, Neutral; 5, Strongly agree. [b]Scale range for Q3: 1, Very difficult; 3, Neutral; 5, Very easy. [c]Scale range for Q4: 1, Very unlikely; 3, Neutral; 5, Very likely. [d]Scale range for Q5: 1, No interest; 3, Neutral; 5, Very keen.

objectives from their prior learning, and integrate and apply knowledge interchangeably between various modules. This also informed the students on a wider range of programming skills used in the industry and preparing them for Industry 4.0.[20]

CONCLUSION

Through this activity, Chemistry or Chemical Engineering undergraduates would be introduced to the basics of Computer Science while conducting an experiment familiar to them. Integrating the use of enabling technologies into such experiments provided an opportunity for students to broaden their perspectives in this subject, and understand the interdisciplinary nature of science. Given that Python is an open-source programming language, with a myriad of learning resources available online, interested students would be able to pursue this topic outside the classroom in their own time should they desire.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.9b00802.

Example brief descriptions with file formats indicated are shown below; customize for your material; installation instructions to setup Anaconda in Windows, with the additional Pyserial and Pyautogui packages, materials and methods (PDF, DOCX)

Full Python code for the visual-aided automated titrator (TXT)

Video of the demonstration (MP4)

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Notes

The authors declare no competing financial interest.

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REFERENCES

(1) Bernlind, C.; Urbaniczky, C. An efficient laboratory automation concept for process chemistry. *Org. Process Res. Dev.* **2009**, *13* (6), 1059−1067.

(2) Pan, J. Y. Engineering chemistry innovation. *ACS Med. Chem. Lett.* **2019**, *10* (5), 703−707.

(3) Kelly, J. M. Panel discussion: Problems on automation of chemical analysis and industrial process. *Ann. N. Y. Acad. Sci.* **1960**, *87* (2), 944−951.

(4) Milo, A. The art of organic synthesis in the age of automation. *Isr. J. Chem.* **2018**, *58* (1−2), 131−135.

(5) (a) Sanderson, K. Automation: Chemistry shoots for the moon. *Nature* **2019**, *568*, 577−579. (b) Steiner, S.; Wolf, J.; Glatzel, S.; Andreou, A.; Granda, J. M.; Keenan, G.; Hinkley, T.; Aragon-Camarasa, G.; Kitson, P. J.; Angelone, D.; Cronin, L. Organic synthesis in a modular robotic system driven by a chemical programming language. *Science* **2019**, *363* (6423), eaav2211. (c) Li, J.; Ballmer, S. G.; Gillis, E. P.; Fujii, S.; Schmidt, M. J.; Palazzolo, A. M. E.; Lehmann, J. W.; Morehouse, G. F.; Burke, M. D. Synthesis of many different types of organic small molecules using one automated process. *Science* **2015**, *347* (6227), 1221−1226. (d) Jiang, T.; Bordi, S.; McMillan, A. E.; Chen, K.-Y.; Saito, F.; Nichols, P.; Wanner, B.; Bode, J. An integrated console for capsule-based, fully automated organic synthesis. *ChemRxiv* **2019**; https://doi.org/10.26434/chemrxiv.7882799.v1.

(6) Fitzpatrick, D. E.; Battilocchio, C.; Ley, S. V. Enabling Technologies for the Future of Chemical Synthesis. *ACS Cent. Sci.* **2016**, *2* (3), 131−138.

(7) Ahneman, D. T.; Estrada, J. G.; Lin, S.; Dreher, S. D.; Doyle, A. G. Predicting reaction performance in C-N cross-coupling using machine learning. *Science* **2018**, *360* (6385), 186−190.
(8) Granda, J. M.; Donina, L.; Dragone, V.; Long, D.; Cronin, L. Controlling an organic synthesis robot with machine learning to search for new reactivity. *Nature* **2018**, *559*, 377−381.
(9) Holme, T. A. Can today's chemistry curriculum actually produce tomorrow's adaptable chemist? *J. Chem. Educ.* **2019**, *96* (4), 611−612.
(10) Hill, M. A.; Overton, T. L.; Thompson, C. D.; Kitson, R. R. A.; Coppo, P. Undergraduate recognition of curriculum-related skill development and the skills employers are seeking. *Chem. Educ. Res. Pract.* **2019**, *20* (1), 68−84.
(11) Kockmann, N. Digital methods and tools for chemical equipment and plants. *React. Chem. Eng.* **2019**, *4* (9), 1522−1529.
(12) Ley, S. V.; Ingham, R. J.; O'Brien, M.; Browne, D. L. Camera-enabled techniques for organic synthesis. *Beilstein J. Org. Chem.* **2013**, *9*, 1051−1072.
(13) Solana-Altabella, A.; Sánchez-Iranzo, M. H.; Bueso-Bordils, J. I.; Lahuerta-Zamora, L.; Mellado-Romero, A. M. Computer vision-based analytical chemistry applied to determining iron in commercial pharmaceutical formulations. *Talanta* **2018**, *188*, 349−355.
(14) (a) Stock, J. T. An apparatus for demonstrating automatic potentiometric titration. *J. Chem. Educ.* **1966**, *43* (8), 425−427. (b) Hernlem, B. J. A versatile and economical automated titration apparatus. *J. Chem. Educ.* **1996**, *73* (9), 878−881. (c) Mak, W. C.; Tse, R. S. Microcomputer automation of volumetric titration. *J. Chem. Educ.* **1991**, *71*, 965−966. (d) Hopkins, H. P.; Hamilton, D. D. Innovations in pH Titrations: Introduction to Automation and Data Analysis with a PC in a Physical-Analytical Laboratory. *J. Chem. Educ.* **1994**, *68*, A95. (e) Famularo, N.; Kholod, Y.; Kosenkov, D. Integrating chemistry laboratory instrumentation into the industrial internet: Building, programming, and experimenting with an automatic titrator. *J. Chem. Educ.* **2016**, *93* (1), 175−181. (f) Soong, R.; Agmata, K.; Doyle, T.; Jenne, A.; Adamo, A.; Simpson, A. J. Rethinking a timeless titration experimental setup through automation and open-source robotic technology: Making titration accessible for students of all abilities. *J. Chem. Educ.* **2019**, *96* (7), 1497−1501.
(15) Bell, S. The role of automated instrumentation in undergraduate Chemistry. *J. Chem. Educ.* **2000**, *77* (12), 1624−1626.
(16) Weiss, C. J. Perspectives: Teaching chemists to code. *Chem. Eng. News* **2017**, *95* (35), 30−31.
(17) Python Software Foundation. *Python Language Reference*, ver. 3.7; http://www.python.org (accessed 2020-01-25).
(18) Python Software Foundation, *Pyserial*, ver. 3.4; https://pypi.org/project/pyserial/ (accessed 2020-01-25).
(19) Python Software Foundation, *PyAutoGUI*, ver. 0.9.48; https://pypi.org/project/PyAutoGUI/ (accessed 2020-01-25).
(20) Teles dos Santos, M.; Vianna, A. S., Jr.; Le Roux, G. A.C. Programming skills in the industry 4.0: are chemical engineering students able to face new problems? *Educ. Chem. Eng.* **2018**, *22*, 69−76.

https://dx.doi.org/10.1021/acs.jchemed.9b00802
J. Chem. Educ. 2020, 97, 850−854