Implementation of LabVIEW for Computer-Controlled Experiments in General Chemistry Laboratory Instruction

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Abstract: A case is made for the pedagogical advantages of standardizing on LabVIEW-based computer-controlled experiments in introductory chemistry laboratory instruction. Experiments already in use, some for several years, in courses with large enrollments are described.

Introduction

The section on Laboratory Work in Chemistry in the latest edition of *Undergraduate Professional Education in Chemistry: Guidelines and Evaluation Procedures*, published by the American Chemical Society [1], states, "Laboratory instruction should include practical experience with instrumentation for spectroscopy, separation techniques, electrochemical methods, and computerized data acquisition and analysis;" yet, a comparison of the syllabi of introductory chemistry lecture and laboratory courses reveals that a nineteenth century chemist would be ill-at-ease with some of the most important material in the lecture course but very comfortable with almost all the material in a typical laboratory course [2]. We wish to show that extensive use of computers in introductory chemistry laboratory courses provides opportunities for closer tracking of lecture and laboratory syllabi, in addition to offering several other major advantages.

The effectiveness of computers as tools in education is still the subject of hot debate [3, 4]. All teachers and administrators in higher education should be required to read "The Soul of a New University," a provocative OP-ED column in *The New York Times* of March 13, 2000 by Arthur Levine, President of Teachers College, Columbia University [4].

Specifically in chemistry undergraduate education, there is no firm experimental evidence for learning being enhanced as a result of the introduction of computers. Still, with respect to undergraduate laboratory instruction, we can bypass this debate by invoking some common sense. The occasional comment that the introduction of computers into freshman chemistry laboratories is "overkill" can be addressed with an analogy: After television became ubiquitous in homes, there were predictions that TV would also become a powerful education tool, but it did not happen; however, there has never been any debate about the need for television equipment in laboratory work for telecommunications majors. In the same vein, the computer has been a fixture of chemistry research and the chemical industry for a long time, and its absence from the freshman chemistry laboratory deprives students of the opportunity to learn much real-world chemistry. Some examples are presented below.

Aside from psychological factors, a major cause of the slow pace for the introduction of computers into freshman chemistry instruction has been cost. We will show below that freshman chemistry laboratory instruction with computers is not only pedagogically more versatile and flexible than without them, but that it is also lowers the cost of required equipment.

We have had several years of experience with the use of LabVIEW-based computer-controlled experiments in freshman chemistry laboratory instruction. Some specific instances of LabVIEW-based experiments in introductory chemistry laboratory courses have been reported by others [5–7]. This article is an attempt to share the details of our experience, to make it easier for others to implement similar programs, and to make some predictions about future trends.

Why Computer-Controlled Experiments and Why LabVIEW?

Even though our motivation for introducing computer-controlled experiments has been pedagogical, as described below, in the real world economic considerations often trump pedagogy. The equipment budget for LabVIEW-based experiments is actually lower than for experiments done without computers. The cost of one suitable PC plus a pH transducer plus a three-frequency colorimeter transducer (see below) plus interface hardware (see below) is less than the cost of one suitable pH meter plus one suitable spectrophotometer. For example, instead of each student having to use a relatively expensive pH meter, with its fixed knobs and dials, that student can use a $72 pH transducer [8] connected to an interface board on a PC in the laboratory. Furthermore, the required space for the many pH meters, many spectrophotometers, etc. is greater than for the PCs plus the small transducers (Figure 1). Details are presented under "Hardware".

To begin our discussion of the pedagogical aspects of using this software in the laboratory, it is pertinent to quote E. K. Wilson: "When computers take over the dirty work in college chemistry labs, students can focus on the bigger picture [9]." Computers allow more variety and sophistication in data collection and analysis. For example, fast data acquisition becomes easy, expanding the range of kinetic experiments [10]. Our ability to create virtual instruments, as described below, gives us unlimited capabilities for creating and modifying the way students do their data acquisition and analysis. Refinements can be made very quickly as we observe student performance and get student feedback. LabVIEW is a high-level graphical programming environment invented and sold by National Instruments for the purpose of creating computer-controlled measurement and automation tasks

Figure 1. Colorimeter sensor unit from Vernier Software [8].

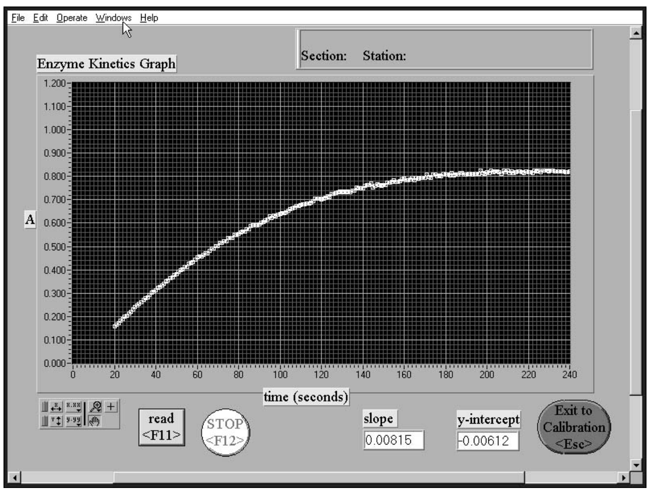

Figure 2. LabVIEW virtual-instrument screen, pictured at the end of the enzyme kinetics experiment [10].

Figure 3. Routing box for analog transducers.

LabVIEW is used in mission-critical applications in industry. National Instruments is the "Microsoft" of computer-controlled measurement and automation. Hence, LabVIEW is not likely to become a dead-end development platform. Compiled LabVIEW run-time executables run license-free on the student stations. LabVIEW based computer-controlled experiments provide the following set of advantages over conventional experiments: (a) They offer less cookbooking and more opportunities that allow students to do experiments that emulate real research and chemical analysis. (b) LabVIEW virtual-instrument panels are software modules that can be easily reprogrammed to suit a variety of experiments in contrast to the fixed knobs and switches on pH meters, spectrophotometers, etc. (c) Students can learn real-world record-keeping techniques instead of using medieval record keeping. (d) Students get better training for the world in which they will inevitably live and work.

An example may illustrate the points presented above. The spectroscopy module for our enzyme kinetics experiment [10] is a small $99 transducer (Figure 1). The experiment would be frustrating and almost impossible if the spectroscopic monitoring (every few seconds) had to be done manually. Instead, a LabVIEW virtual instrument software module built by us and described under "Software Considerations" and shown in Figure 2 does the monitoring [10].

Why LabVIEW instead of computer-contolled experiments based on commercially available hardware interfaces and software specifically designed for undergraduate instruction? The first advantage of LabVIEW is its robustness and its guarantee of availability for major operating systems of the future; LabVIEW is the de facto standard for computer-control and automation in mission-critical industrial applications. Second, we the users create the LabVIEW virtual instrument software modules, and we the users can easily modify them. Third, the cost of the required hardware interfacing is typically lower for the LabVIEW choice; mass production does lead to lower prices. This will be discussed further in the section on "Hardware Issues."

If, as we demonstrate, there is a pedagogical upside and an economic upside to the use of LabVIEW-based computer-controlled experiments in introductory chemistry laboratories, is there any downside? One possible downside is the learning curve for LabVIEW programming by a professor or co-worker. Fortunately, LabVIEW is an easy high-level graphical programming language that involves connecting graphical elements on the PC screen. This will be discussed further in the section on "Software Issues". Another possible drawback is that computers may hide an educationally valuable real-world occurance: unreliable instrument conditions that students might encounter using manual control.

Hardware Issues

LabVIEW software is available for many operating systems including the Mac OS and Windows 98/NT. Our own experience is only with Intel-based computers. All hardware and software issues discussed here refer to Intel-based PCs running Windows NT 4.0 and to a lesser extent Windows 98.

There is a cost involved in being able to send to the computer the analog or digital signal produced by a transducer or instrument. There are several connection points available at the computer, and purchasing decisions are not easy now because of rapidly changing interface options. The more traditional options involve boards for the ISA bus (almost defunct), boards for the PCI bus (thriving), and the serial port (zero cost, if the chemical instrument has a serial port). A newer option available on all PCs manufactured in the last few years is the Universal Serial Bus (USB), which, in principle, is the most attractive option [11], but in practice has some drawbacks at this time, as described below.

The simplest input is the serial port, which is supported by the LabVIEW software. It is relatively slow (up to 115 kbits/s typically), but fast enough for all our needs in introductory chemistry. It is directly usable with relatively expensive

Figure 4. A laboratory in session.

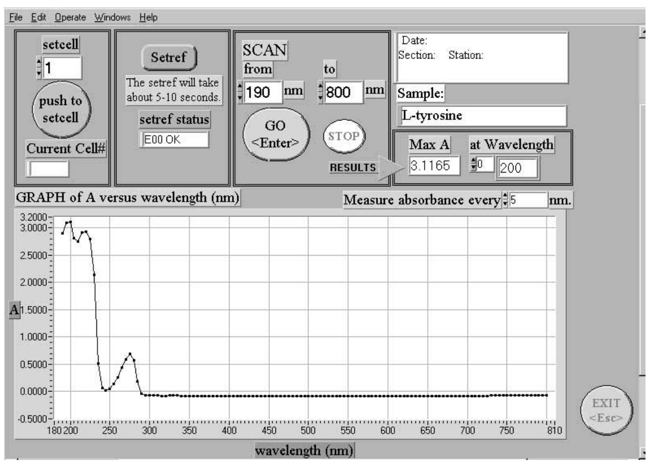

Figure 5. LabVIEW screen at the end of a full-range electronic spectroscopy scan of a sample of aqueous tyrosine on the Ultrospec 2000. The spectrometer is totally under LabVIEW control. The scale ranges are adjustable with the mouse and keyboard.

instruments that have a serial port, such as the Ultrospec 2000 spectrophotometer from Pharmacia Biotech. It is not practical for inexpensive analog transducers (pH, fixed-frequency spectrophotometry, temperature, etc.), because it would require an A/D interface box for the serial port, an unattractive option in comparison to others described below.

The most attractive option is, in principle, the Universal Serial Bus [11]. There are two USB ports on most PCs that have been built recently. USB allows hot-swapping (connection and disconnection of devices without shutting down the computer), a major advantage for the many laboratories and laboratory sessions involved in large-enrollment courses. Up to 127 USB devices can be daisy-chained, at least in principle. Following the lead of the Apple iMac, some PC manufacturers are already moving in the direction of using the USB port for all common external devices and deleting the parallel port, serial port, keyboard port, and mouse port. The USB port is fast; under the current USB version 1.1 specification, full-speed USB devices signal at 12 Mbit/s (1.5 MB/s) while low-speed devices use a 1.5 Mbit/s subchannel [11]. The new USB 2.0 specification, under development [11], will support speeds up to 480 Mbit/s (60 MB/s), fast enough for a variety of new applications of LabVIEW. The downside? A minor downside for now is that, on the PC side, Windows 98 supports USB but the more robust Windows NT 4.0 does not. The new poorly named Windows 2000 (really NT 5.0) supports USB, but the robustness of the USB support has not been widely tested as of yet. A major temporary downside is cost: A USB data-acquisition box now costs about $900, but prices should fall as USB gets more widely used because of its advantages. For serial interfaces, a low-cost way of taking advantage of USB now is the USB-to-serial adapter. A good one, such as the Belkin model FSU003 [12], sells for less than $60, and it allows us to hot-swap the Ultrospec 2000, for example. It works (under Windows 98).

The most practical general purpose interface, currently, is a PCI-bus data-acquisition board such as the PCI-6023E from National Instruments ($355 educational price) [13] or the PCI-DAS08 from ComputerBoards ($224 educational price) [14]. Each data-acquisition board requires software drivers for LabVIEW. Such drivers are available for all National Instrument boards [13] and for practically every board made by other manufacturers. With prices of adequate PCs plunging to below the $1,000 level, the cost of data-acquisition hardware is still a significant fraction of the investment in large-enrollment environments. For several years our freshman chemistry students have been doing LabVIEW-based experiments on computers equipped with an earlier model of data-acquisition boards from National Instruments. At each PC station, analog devices (pH, fixed-frequency spectrophotometry, temperature) from Vernier Software [8] are connected to a small routing box (Figure 3) built here, which is connected by a cable to the data-acquisition board in the PC. Details are available upon request. Each 24-student freshman chemistry laboratory is equipped with 12 networked PCs; two students share a PC (Figure 4). There is also a networked printer in each laboratory.

Software Issues

LabVIEW virtual-instrument modules such as the ones shown in Figures 2 and 5 are created in the LabVIEW Full Development System, now in Version 5.1, available for numerous operating systems [13]. This software has an educational price of $1,297 for a single development license. In order to create license-free stand-alone virtual-instrument software executables, one must also purchase the Application Builder software for $995. Also, a student edition of LabVIEW 5.0 published by Addison-Wesley [15] is available for $90. It includes a Student Edition of the programming software and a book [16].

Many books on LabVIEW programming are available [16–24], ranging from introductory [16–18] to advanced [19–22] and specialized [23, 24].

It is realistic for someone without any programming experience to learn LabVIEW programming quickly enough to develop virtual instruments for use in introductory chemistry courses. Here we shall present the experience of one of us (Dobie-Galuska), who had no programming experience and no computer expertise prior to learning LabVIEW programming.

1994. I started by doing the LabVIEW tutorial, which provides lessons for running and modifying samples of virtual instrument software modules (VIs) and guidance on how to make some simple VIs. I received some help from

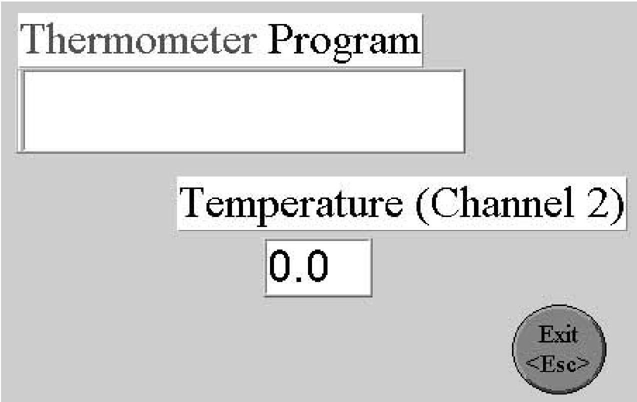

Figure 6. A simple virtual instrument software module for temperature monitoring.

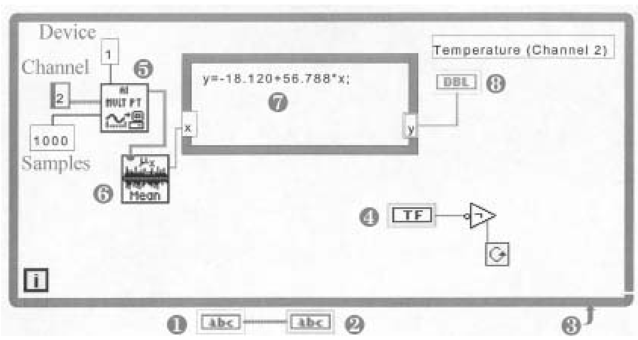

Figure 7. The source code for the VI of Figure 6.

a National Instruments sales representative and from a professor who has programming experience, but mostly I learned LabVIEW programming by reading the tutorial and manuals and trying things out until they worked.

1996. I took the National Instruments LabVIEW Basics and Advanced courses. These courses, which last one week, are offered in a variety of locations [13]. Much of the material that was covered I had already learned on my own, but up to this point I really had no feedback on my LabVIEW programming skills. The engineer who taught the class was impressed by how much I had done on my own.

As an illustration of LabVIEW programming, Figure 6 shows a simple VI for temperature measurements, and Figure 7 shows the source code for this VI.

Items 1–8 of Figure 7 are: **(**1) string control that brings in student and date information entered in a screen previous to that of Figure 6; (2**)** string indicator that displays student and date information; it is blank on the screen of Figure 6 because no data has been entered; (3) “while” loop; tells computer to run what is inside the loop until the loop is “exited;” (4) exit button; when pushed sends a false command to the while loop, which ends the loop. (5) LabVIEW VI subroutine from National Instruments called “AI Acquire Waveform.vi” that manages the data acquisition; it must be told which device and channel to collect data from, as well as how many samples to collect; (6) LabVIEW VI subroutine from National Instruments called “mean.vi” that computes the mean of values “wired” into it; in this case it calculates the mean of the 1,000 samples of acquired data from “AI Acquire Waveform.vi;” (7) formula node programmed to convert mean reading from volts (x) to ^{o}C (y); the conversion equation from manufacturer of temperature probe can be verified by calibration. (8) digital indicator that displays the temperature; the number of displayed digits can be chosen.

Most of the programs I have written are variations of one program. The basic program collects some analog data from a probe (in volts) through the data-acquisition board and then translates the volts to another unit such as pH. The code or diagrams for many of the features that I have included in my programs come directly from the example VIs that are supplied in LabVIEW. Indeed one programming strategy that was encouraged at the class I took was to find an example VI and modify it to suit your purpose. It is even possible to modify some of the function VI subroutines that are supplied as part of the LabVIEW code. For instance, I have modified a function VI that manages saving to a spreadsheet file. My modification was to make the program include a heading with the student’s name, the date, and the experiment title as well as labels for the columns of data. Without this modification the data would be saved as just two columns of numbers.

I wrote one program that interfaces an instrument, the Ultrospec 2000, through the serial port rather than through the data-acquisition board (Figure 5). I was able to obtain the serial commands for the Ultrospec from Pharmacia technical support. Within a month I learned how to use the serial VIs in LabVIEW and made a program that could have a conversation with the Ultrospec.

Specific Experiments

All the LabVIEW-based experiments listed below, except the first two, are described in detail in the 5th edition of *The C125 & C126 Laboratory Manual* authored by R. A. D. Wentworth and A. A. Dobie-Galuska [25].

Introduction to Bioanalytical Electronic Spectroscopy. Students learn the fundamentals of electronic spectroscopy by recording and comparing the electronic spectra of ethanol, L-lysine, L-tyrosine (Figure 5), phenolphthalein at neutral pH, phenolphthalein at high pH, beet juice, and hemoglobin. These experiments introduce the concept of chromophores and will prepare the student for the applications of electronic spectroscopy described below. The spectra, recorded on the Ultrospec 2000 (Figure 5), will serve as springboards to the concepts of energy levels, electronic energy levels (σ, σ*, π, π*), interaction of light with molecules; absorption spectroscopy, electronic spectroscopy ($\sigma \rightarrow \sigma$* and $\pi \rightarrow \pi$* transitions), chromophores for $\sigma \rightarrow \sigma$* and $\pi \rightarrow \pi$* transitions (and specific molecules), effect of conjugated double bonds on $\pi \rightarrow \pi$* transitions (with examples), UV and visible spectra, and the color wheel (absorbed color vs. observed color). Details will be published elsewhere.

Bioanalytical Applications of Electronic Spectroscopy. As a sequel to the preceding experiment, students evaluate two methods, both based on electronic spectroscopy, to determine protein concentrations. One method takes intact protein solutions and uses the $\pi \rightarrow \pi$* transitions of aromatic amino acid residues in the ultraviolet region of the spectrum. The other method involves a chemical modification of the protein that yields an absorption in the visible region of the spectrum. Students are charged with evaluating the merits and drawbacks of each method for specific types of applications in research and industry. Specifically, they use both methods to determine concentrations of protein in milk whey from buttermilk and in solutions of gelatin. The spectra, recorded on the Ultrospec 2000 (Figure 5), will serve as springboards to student research on primary structure of proteins, structures of amino acid side chains, amino acid backbone and side chains as chromophores in electronic spectra, variations in amino acid composition (bovine lactalbumin and gelatin), examples of electronic spectra of amino acids (review of preceding experiment), chemistry of the Biuret reaction, and prediction of spectrum and color of Biuret-modified protein. Details will be published elsewhere.

Enzyme Kinetics. The enzyme kinetics experiment uses the spectrophotometer sensor of Figure 1 and the virtual instrument module of Figure 2. Details have been published [10].

Equilibrium Constant. Students determine the equilibrium constant for the reaction

$$Fe^{3+}(aq) + SCN^{-}(aq) \rightleftharpoons Fe(SCN)^{2+}(aq)$$

spectrophotometrically, by taking advantage of the strong $Fe(SCN)^{2+}$ absorption at 450 nm.

Strengths of Acids and Bases. These are titration experiments that use the pH electrodes from Vernier Software [8] connected to one of the inputs of the routing box (Figure 3).

Acid–Base Titrations. These are more titration experiments that use the pH electrodes from Vernier Software [8] connected to one of the inputs of the routing box (Figure 3).

Buffer Solutions. These are still more titration experiments that use the pH electrodes from Vernier Software [8] connected to one of the inputs of the routing box (Figure 3).

Thermochemistry and Hess's Law. The temperature of a reaction mixture is monitored over time, using a Vernier [8] temperature probe. The goal of the experiment is to determine the heat of reaction of an acid–base reaction and the heat of solution of a salt. This determination is done both by experiment, using calorimetry, and by calculation, according to Hess's Law. A coffee-cup calorimeter is used to measure the temperature change that occurs with the acid–base reaction and with the salt dissolution. The initial temperature for both processes is measured before the reaction or dissolution is begun using a simple VI that measures temperature (Figures 6 and 7). Another sub-VI measures and plots temperature over time.

Spectrophotometric Determination of Molar Concentration. The goal of this experiment is to determine the concentration of a food dye solution. The students prepare standard solutions and construct a plot of absorbance versus concentration. The resulting molar absorptivity constant is used to determine the concentration of an unknown solution. Before making the absorbance measurements for the standard curve, the students run a scan of their food coloring sample to determine the wavelength that gives the maximum absorbance. The Ultrospec 2000 is used to make the absorbance readings for the scan (as in Figure 5). Students can watch this scan develop on the screen. They can print it when it is complete. A Vernier [8] colorimeter (Figure 1) is used to measure absorbance of the standard samples at the maximum wavelength. A computer program is used that collects the absorbance data and also allows the students to input the concentration of the standard solutions. The program, therefore, can show a plot of absorbance versus concentration on the screen during the experiment. The students open the absorbance and concentration data within Excel to create their own plot and determine the slope (molar absorptivity constant). It is possible to have the LabVIEW VI determine the slope, but we chose to have the students do their own analysis.

Conclusions

As we mentioned at the beginning of this article, the section on Laboratory Work in Chemistry in the latest edition of *Undergraduate Professional Education in Chemistry: Guidelines and Evaluation Procedures* [1] states: "Laboratory instruction should include practical experience with instrumentation for spectroscopy, separation techniques, electrochemical methods, and computerized data acquisition and analysis." If the implementation of these goals is to start in the freshman year, as we believe it should, then the LabVIEW-based computer-controlled systems described in this article should facilitate such implementation.

We have made a case for the pedagogical and practical advantages of LabVIEW-based computer-controlled experiments in introductory chemistry laboratory courses. The range of feasible and affordable experiments (such as fast kinetics and spectroscopy) is increased, allowing for greater correspondence between lectures and the student's laboratory experience. As computers and data-acquisition interfaces become more versatile and less expensive, as they inevitably will, the trend towards computer-controlled experiments in introductory chemistry instruction will accelerate. Students who are science majors will benefit from experiences more closely related to their future real-world work. All students will benefit from the experience of data acquisition and analysis by computer. There is also an opportunity to train advanced undergraduates and graduate students in the creation of LabVIEW-based computer-controlled experiments by having them learn to use the student edition of LabVIEW [15].

Finally, we will be happy to share our experiences, our compiled virtual instruments, and our source code.

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