Virtual Instruments in an Undergraduate Environmental Engineering Laboratory

Monroe L. Weber-Shirk, Leonard W. Lion
Cornell University

Abstract

Cornell's School of Civil and Environmental Engineering (CEE) is developing a new undergraduate laboratory course in Environmental Engineering. This course includes innovative experiments related to recent or ongoing research conducted by CEE environmental faculty.

A goal during course implementation was to integrate computerized instrument control and data acquisition without making computers and software the course focus. This would enable students to concentrate on theory and application of physical, chemical, and biological processes with minimal time spent learning how to use new software packages or instruments.

To achieve these goals in a cost effective and timely manner we developed customized "Virtual Instruments" (VIs) with a similar design for multiple instruments. Software was written using LabVIEW™ to control and acquire data from a UV-Visible spectrophotometer, a gas chromatograph, a 3-axes positioning system, and a pH-ion meter that was also used to measure conductivity and dissolved oxygen.

The first semester of student use in both the new undergraduate environmental laboratory course and a graduate level laboratory course confirmed the value of the new computerized instrumentation. While in the laboratory, students were able to monitor time varying processes and perform data analyses that previously were not feasible. The features of VI's that were developed for student use are discussed in this paper.

Introduction

Laboratory experience is a crucial element in the education of engineers. However, implementation of successful undergraduate engineering laboratory programs is hampered by inadequate and antiquated equipment, lack of appropriately equipped space, and inadequate participation of qualified engineering faculty. Until recently these obstacles had prevented Cornell's School of Civil and Environmental Engineering from offering an undergraduate course in Environmental Engineering. However, strong interest from the faculty combined with institutional support and funding from industry and National Science Foundation have made it possible to create a new undergraduate laboratory course in Environmental Engineering.

Creation of the new course provided opportunity to consider alternatives for course design and implementation. Our goals were:

to provide an educational environment in which students with different learning styles could interact with the course material in different ways .

to develop laboratories that illustrate current environmental issues and provide a context for teaching

fundamental theories and analytical techniques.

to help students develop an intuition for various environmental engineering processes.

to teach students the skills necessary to perform laboratory work.

to give students hands-on experience using modern instrumentation.

to give students a taste of the excitement and challenge of research.

to provide an environment where students can develop their problem solving skills (especially when the real world doesn't seem to fit with theory).

to minimize the drudgery of repetitive tasks.

Several of the above goals suggested use of computerized data acquisition would be highly desirable. We considered computerized data acquisition because many of the laboratory exercises dealt with time varying processes, and development of instrumental controls with a common user interface could facilitate increased student focus on the manifest purpose of each lab and reduce attention given to instrument operation and data analysis. Previous implementations of computerized data acquisition and control in undergraduate laboratories have often necessitated inclusion of several weeks of instruction to introduce the students to the computer system. However, we did not want computers to become the focus of the course. Thus we wanted to develop software that could be used by students with minimal additional training. Ideally the software would significantly decrease the amount of time students required to learn how to use a new instrument.

Given the time constraints for development of data acquisition software we initially considering a gradual implementation after the course was underway. However, experiments performed with and without computerized data acquisition are often designed differently and thus gradual implementation of computerization would have required an additional effort to convert experimental designs. In addition, the instruments chosen for use in the laboratory needed to be selected carefully to ensure compatibility with computerized data acquisition.

Thus, we chose to develop laboratory modules that included computerized data acquisition as an integral part of the initial laboratory development. The major impediment to implementation of computerized data acquisition was the possibility that it might significantly prolong the course development time. The tool that made it possible to develop the data acquisition software in a timely manner was the use of Virtual Instruments.

Virtual instruments (VIs) move instrument control from the instrument panel to the computer. This permits development of a customized, consistent user interface for a wide array of instruments. The instrument-specific aspects of analyses can be minimized allowing students to focus more on the data and the process. The features of the VIs that have been developed to date are described below.

Careful selection of instruments with text-based communication (serial port or GPIB interface) was also a factor contributing to a short development time. This eliminated the need to monitor analog signals. Instruments with serial port or GPIB communication capabilities often can be controlled through the communication interface and thus VIs with full instrument control handled by the computer can be developed.

Hardware and software development environment

We chose LabVIEW™ running on Power Macintosh computers as the development platform for the instrumental analysis/data acquisition software. However, similar results could be obtained with other platforms using the same software. The instruments selected provide options for both computerized data acquisition and instrument control and include: pH-ion meters, gas chromatographs, diode array UV-Vis spectrophotometers, and a 3-axis positioning system.

The pH-ion meter, gas chromatograph, and 3-axis positioning system use serial port communication and the spectrophotometer relies on a GPIB interface. Thus the only instruments that required additional data acquisition hardware (a GPIB interface board) were the spectrophotometers. Although cables designed to connect the Macintosh serial ports to the gas chromatograph, pH-ion meter, and 3-axis positioning system are not commercially available, custom cables for each of the instruments were fabricated by cutting Macintosh printer cables in half and splicing the cut ends to the appropriate connectors for each instrument.

Serial port communication proved to be an excellent choice for the processes monitored in our laboratory. Serial port communication allows the computers to perform multitasking with minimal risk of data loss. If the computer is busy with other tasks the serial port buffer can accumulate the data until computer processor time is again given to the VI.

Virtual Instruments

LabVIEW™ (National Instruments) was chosen as the software development environment because it has a full featured graphical interface designed for instrument control, data acquisition, and analysis. Software development requires a significant investment of time and it was necessary to develop low level communications protocols, appropriate data analysis, and a user interface for each instrument. Many of the time consuming programming tasks typically required to develop a user-friendly interface are taken care of by high level LabVIEW™ features including full featured graphical displays (for example, built in graphs have the ability to autoscale, zoom, format axis, etc.) and extensive data handling and data analysis capabilities.

To the extent possible the user interfaces for the various VIs were designed to look the same. Each interface features a simple control panel that presents the basic options available. The consistent interface design helps students quickly learn how to use new instruments. The similarity in the user interfaces is also mirrored by similarities in the underlying code which reduced the time required to develop the VIs.

pH-Ion meter

Selection of instruments that have multiple functions was used to add additional capability to the laboratory without significantly increasing programming time. This economy was realized by careful selection of a pH-ion meter. The Accumet™ 50 pH-ion meter (Denver Instruments) was selected because it provided the capacity to simultaneously monitor two pH probes and one temperature probe. The meter could also be used with a conductivity probe and dissolved oxygen could be monitored by using a special probe (Orion Research, model 5058-1000-2B) designed to be monitored with a pH meter. Thus, once software was written to monitor pH, it was relatively easy to augment the code to monitor conductivity and dissolved oxygen.

Most pH meters have a simple display of the current pH. This is adequate when the goal is measure the pH of a stable sample. However, we were interested in monitoring time dependent variations in pH, conductivity and dissolved oxygen. In the laboratory exercises pH is measured in simulations of the effects of acid rain input on lakes, conductivity is used to monitor the concentration of a conservative tracer in reactors, and dissolved oxygen (D.O.) is used to monitor the effects of biochemical oxidation of organic matter. Each of these processes is time dependent in the student laboratory exercises and thus we desired a real-time graphical display of each parameter.

The Accumet™ 50 pH-ion meter can be controlled via the serial port and user-friendly dialog boxes were created to select the type of probe (pH, conductivity, or D.O.) and the sample rate. However, full control of all of the pH-ion meter's capabilities would have required an excessive amount of code and thus only the most commonly used features were incorporated into the VI.

The pH-ion meter has internal software that gives the instrument several levels of menus. The pH-ion

meter is controlled by sending "keystroke" commands that duplicate the commands that a user could potentially give the meter by using the instrument keypad. Effective computer control of the meter requires the ability to either place the meter in a known state (for example in a measure pH mode rather than a standardize mode) or receive information from the meter that identifies its current state. Unfortunately, the meter does not have the ability to be forced to a given state or to tell the computer what its current state is. The pH-ion meter display prompts the user with screen messages to select appropriate keypad choices, however, these screen messages can not be transmitted to the Virtual Instrument and thus the VI is forced to control the meter blind (without any feedback as to the response of the meter).

As a partial solution to this problem two techniques are used to place the pH-ion meter into a known state. A "clear" command is repeatedly sent to the instrument to return it from any nested commands, and a "print" command is used to determine if the meter is monitoring pH, ion, or conductivity on either 1 or 2 channels. After the current state is determined commands are sent to the meter to return it to a state to which further commands can be sent.

A second programming problem common in text based communication is that instrument data communication protocols are often designed to send text to a printer and are not optimal for parsing. The pH-ion meter sends data formatted with variable numbers of spaces between fields. Although this complicates parsing of the data, LabVIEW™ has adequate text processing capabilities to handle the task.

The VI control panel used to control the pH-ion meter is shown in figure 1. When **Set Method** (figure 1) is chosen the dialog box shown in figure 1 appears. The dialog box allows the user to select automatic timed data transmission or manual data transmission (manual data transmission is controlled by pressing a "print" button on the meter). If the option for **automatic timed intervals** is chosen the pH-ion meter is set up to write the current measured values to the serial port at user-specified intervals. Controls are also available to select the type of probe monitored by each of the two channels. After the dialog box is closed multiple commands are sent to the meter to reset the sample number to zero, to enable timed printing of data, to setup the time interval, and to select the appropriate type and number of probes to monitor.

Selection of **Monitor Sample** prepares the instrument to begin sampling. For timed sampling it is usually appropriate to have a well defined beginning to the sampling. If all of the commands necessary to initiate sampling were sent to the meter there would have been a delay of several seconds before the meter actually sent the first data to the computer. To improve the timing a dialog box was created that informs the user when the meter is ready to begin and then when the **OK** button is selected a final single command is sent to the meter to initiate sampling.

While the meter is transmitting data to the computer the VI continually checks the serial port buffer for the next data transmission. When the next data transmission is complete the VI parses the data text, appends the data from each channel (up to three channels of data with one channel per probe) to an array, and graphs the data arrays. During sample monitoring a **Stop Sampling** button appears on the VI that is used to terminate data transmission from the meter. When data transmission is finished the data arrays can be saved to disk as a tab delimited text file that can be read by any spreadsheet program.
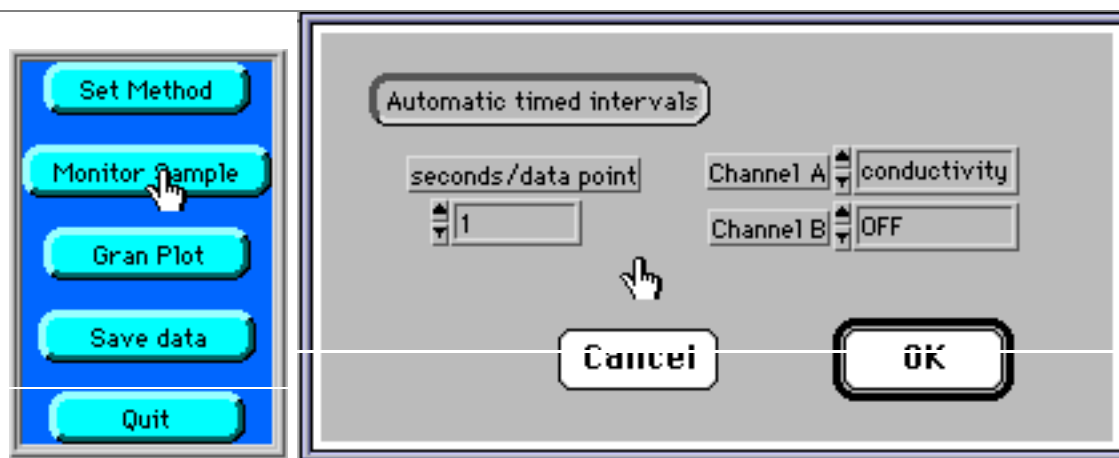
Figure 1.   Control panel (left) and dialog box (right) available under the option of "Set Method" from the VI created for the pH-ion meter. For titrations manual sampling is used while for monitoring a process timed sampling ("Automatic timed intervals") is chosen.

An additional feature required for one of the experiments was the ability to titrate samples to measure their acid neutralizing capacity with data reduction using a Gran plot. The use of VIs made it easy to further customize the software and add this feature. A section of the display showing the titration of sodium carbonate with acid and the resulting Gran plot are shown in Figures 2 and 3. With this addition to the VI students were able to analyze their titration data directly during the laboratory exercise.
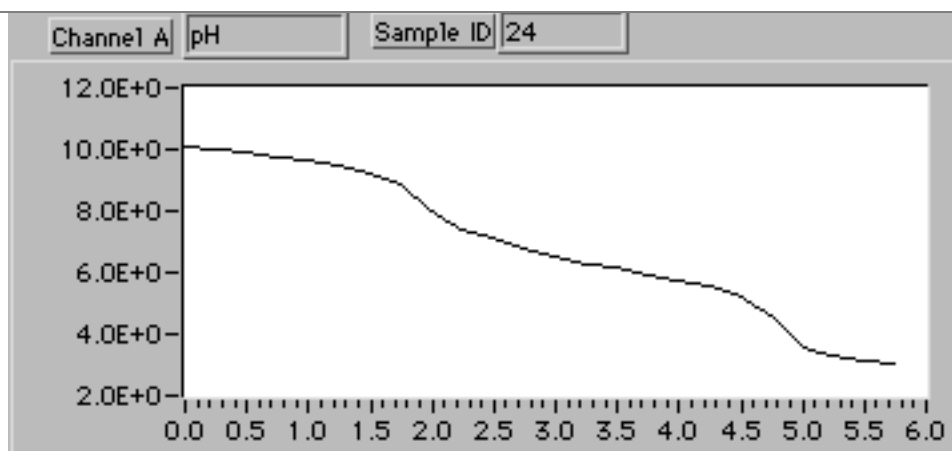

Figure 2.   Graph from the titration of Na_2CO_3 with HCl. The x axis has units of mL of titrant and the y axis is pH.
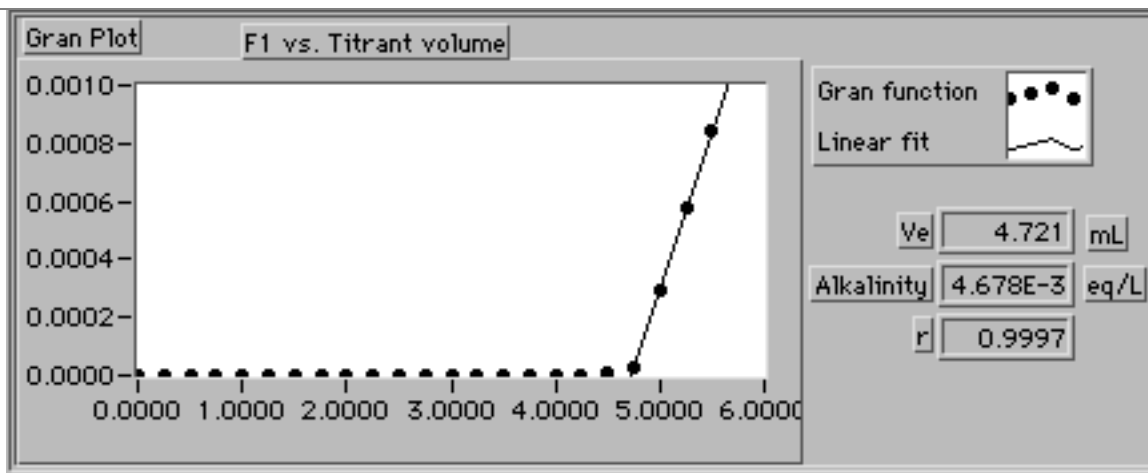
Figure 3.   Gran plot from the titration of Na_2CO_3 with HCl. Gran plot analysis is used to measure the alkalinity (or acid neutralizing capacity) of a sample. The x axis has units of mL of titrant and the y axis is a Gran function with units of $[H^+]$.

Gas chromatograph

The Hewlett-Packard model 5890 Series II gas chromatograph was selected for use in this laboratory. The VI controlling the gas chromatographs provides basic features essential for gas chromatography including control of oven, detector, and injector temperatures and integration of peak areas. Chromatograms can be saved for later analysis or the peak areas can be exported for analysis in a spreadsheet.

For the gas chromatograph VI the following options are available: **Set Method**, **Measure Sample**, **Integrator Settings**, **Save Chromatogram**, **Open Chromatogram**, **Copy Results to Clipboard**, **Print Chromatogram**, and **Quit**. **Set Method** allows the user to set injector, oven, and detector temperatures, turn detectors and heaters on and off, select the type and number of detectors (up to two detectors can be monitored simultaneously), and set the data sampling rate. Temperature controls for the gas chromatographs were made more intuitive by using a graphical display of the selected temperature profile (figure 4).

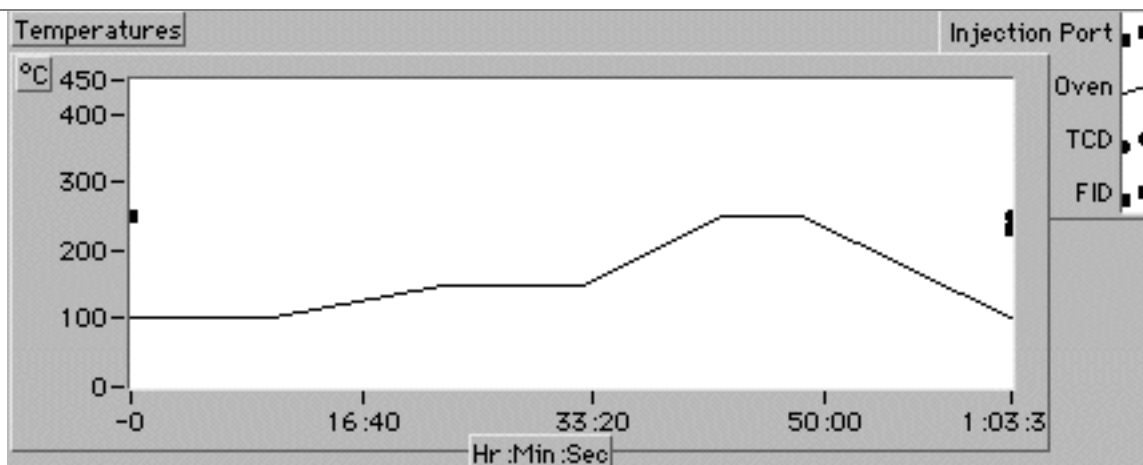1996 ASEE Annual Conference Proceedings

Figure 4.   Graphical display of the gas chromatograph oven temperature profile facilitates changing methods. The selected temperature for the injection port is shown at the left of the graph and the temperatures for the detectors (Thermal Conductivity Detector and Flame Ionization Detector) are shown at the right of the graph.

Measure Sample prepares the gas chromatograph for a sample injection. After sample injection the "Start" button on the gas chromatograph keypad must be pressed to initiate a run and begin transmitting data to the computer. As with the pH-ion meter, the data is processed by the gas chromatograph VI as it is received. In addition, the peak areas are calculated by a peak detection VI obtained from National Instruments. The availability of peak detection/integration software significantly reduced the amount of time necessary to develop data acquisition and control software for the gas chromatographs. The signal, peak start, peak maximum, peak end, and baseline are all plotted in real time (figure 5).
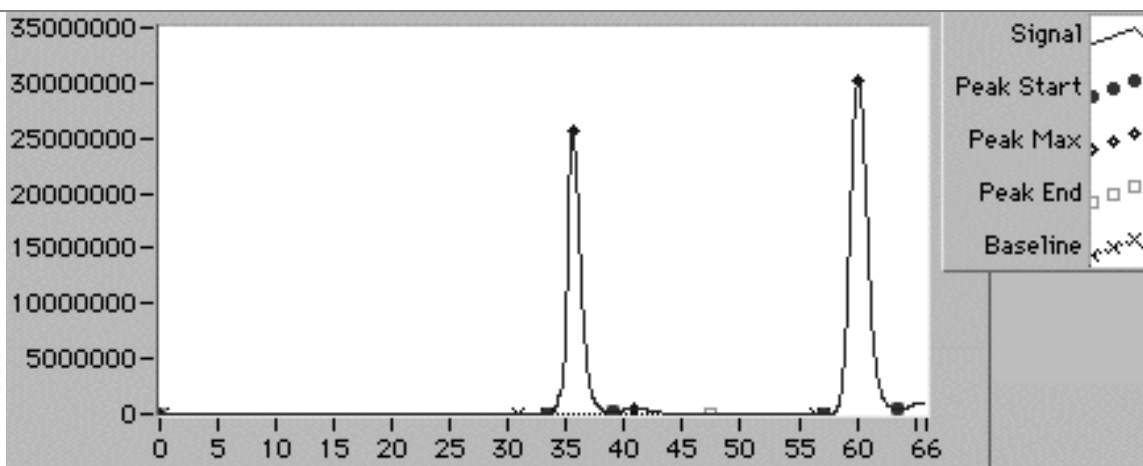

Figure 5.   Example chromatogram obtained from a sample containing hexane and toluene. The x axis is time (sec) and the y axis is the detector signal.

1996 ASEE Annual Conference Proceedings

With the exception of **Quit** the remaining controls available in the gas chromatograph VI do not involve communication with the gas chromatograph. **Integrator Settings** is used to optimize the peak detection VI, **Save Chromatogram** saves the data file as well as user comments to disk, **Open Chromatogram** retrieves a previously saved chromatogram from disk, **Copy Results to Clipboard** places the peak areas and peak times in the computer clipboard and is a convenient way to transfer data to a spreadsheet. **Quit** opens a dialog box that asks the user if the gas chromatograph should be placed in an energy saving mode. If the energy saving mode is selected the heaters and detectors are turned off and the VI releases control of the gas chromatograph.

Diode array spectrophotometer

Diode array spectrophotometers provide absorbance measurements as a function of wavelength. The Hewlett-Packard model 8452A spectrophotometer was selected for use in this laboratory. The spectrophotometer VI handles the tasks of calibration based on standards and analysis of samples of unknown concentration. The absorbance data from both types of samples can be saved to disk for later use. The ability to retrieve previously analyzed standards is especially useful. The Spectrophotometer VI control palette has the following options:

Turn lamp on/off toggles the lamp on and off. After turning the lamp on the lamp intensity is compared with the original intensity of the new lamp. If the lamp is not sufficiently bright the user is alerted.

Measure reference prompts the user for a reference sample which is used to set the zero absorbance level. Taking a sample involves pumping a rinse solution through the sipper cell for a user-selected time and then pumping the sample through the sipper cell for a user-selected time. The VI prompts the user through each step and controls the sipper pump. After the sample is in the sipper cell the VI instructs the spectrophotometer to take a measurement and send the resulting data to the VI. These steps are also used when measuring standards and unknowns.

Measure standards prompts the user for the concentrations of the standards to be analyzed. After the concentrations are entered, the VI prompts the user to sample each standard. The resulting absorbance spectra are displayed on a graph as shown in figure 6. After the standards are analyzed the user is prompted to select a file name and location for the data file.
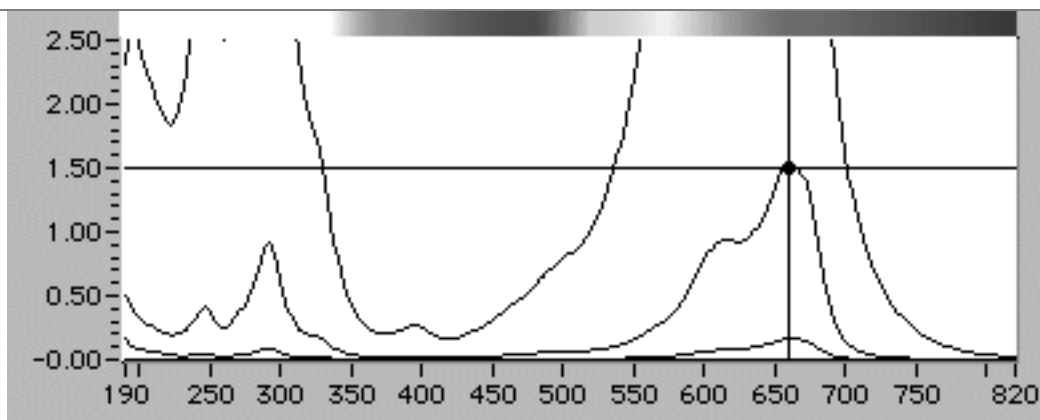

Figure 6.   Example absorbance spectra taken from Spectrophotometer VI showing absorbance of a series of methylene blue standards as a function of wavelength. The x axis is wavelength (nm) and the y axis is absorbance. The crossbar cursor is used to select a wavelength for use in determining the concentration of an unknown. The banded strip at the top of the display shows the visible spectrum corresponding to the wavelength axis.

1996 ASEE Annual Conference Proceedings

Measure unknowns prompts the user to describe the unknowns and then sample each of the unknowns. The resulting absorbance spectra are displayed on a separate graph from the standards. As with the standards, the data file can be saved to disk.

Load standards and **Load unknowns** retrieve previously saved data files from disk for display on the graphs. This makes it possible to reanalyze samples and to reuse standards.

Run pump starts the sipper pump and is used to flush the sipper cell.

Print prints a modified copy of the screen designed for a grayscale printer.

Mixture analysis can be used to measure the concentration of several components of a mixture. If several species are present in a sample the absorbance is simply the addition of the absorbances from the component species. The result of the linear addition of two compounds can be seen in Figure 7. The ability to resolve a mixture into the component species is a function of the shapes of the species' extinction vectors (absorbance as a function of wavelength) and the relative concentrations of the species in the mixture. Extinction vectors tend to have peaks that are many nm wide and different compounds may have extinction vectors that are only slightly different. When the extinction vectors of species are similar the ability to resolve the individual species in a mixture is poor.
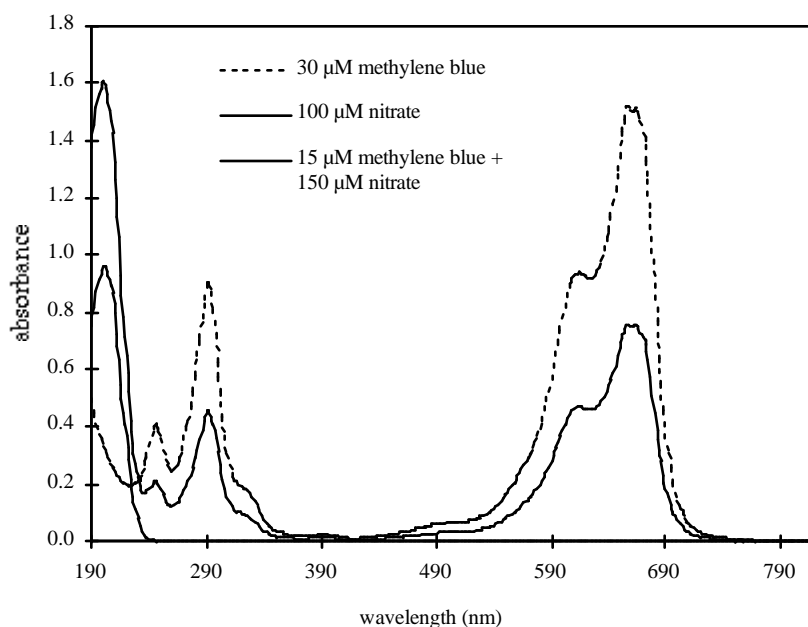

Figure 7. Extinction vectors from methylene blue, nitrate, and a mixture of methylene blue and nitrate.

Mixture analysis occurs as a post-processing analysis that is done after measuring the absorbance of the relevant standards and unknowns. Each of the components of the mixture must first be analyzed as a "standard" and the resulting absorbance spectra saved to disk. Ideally a broad range of concentrations should be analyzed for each "standard." Given a set of standards at differing concentrations, the VI selects the appropriate standard based on the absorbance of the sample and eliminates part of the spectrum if the absorbance exceeds the instrument's linear range. This "autorange" feature makes it possible to analyze samples with a broad concentration range.

1996 ASEE Annual Conference Proceedings

Mixture analysis requires the user to open the relevant data files containing standards and unknowns. The concentrations of each of the standards that would result in the observed absorbance are then calculated using a general least squares fit. The general least squares fit algorithm is available as in the LabVIEW™ analysis package and thus mixture analysis did not require extensive programming.

Continuous sampling runs the sipper pump continuously and measures absorbance at a user-selected time interval. The ability of the spectrophotometer to take measurements rapidly combined with the ability of the computer/software to analyze the data quickly makes it possible to measure the concentrations of a mixture as a function of time. Samples can be taken as frequently as every 2 seconds and analyzed in real time to determine the contribution of each of the selected standards. The component concentrations are graphed as a function of time. The "autoranging" ability of the mixture analysis makes it possible to monitor the changing concentrations in a mixture over a broad range in concentrations. If only one species is to be monitored this same analysis can be used by only selecting the appropriate standard.

Positioning system

A three axes positioning system is used to control the location of a conductivity probe (monitored with the Accumet™ 50 meter) in a laboratory flume. The positioning system is a small trolley that can traverse the length of a flume (x-axis) and has y and z axes to move a probe horizontally and vertically perpendicular to the direction of the water flow. A Velmex model NF90 3-axes controller is used to control three stepper motors. For our application the two Macintosh serial ports are used to control the positioning system and a Accumet™ 50 meter simultaneously. The combined meter/positioning system has the ability to take conductivity measurements along a path, plot the measurements on a graph, and save the data to disk. Some of the code used to control the Accumet™ meter was adapted and included in the positioning system VI.

The positioning system control palette has the following options: **Change velocity…** sets the travel velocities and accelerations for each of the three axes. The relationship between velocity and stepper motor steps for each of the axes can also be changed. **Find home** instructs each of the axes to move in the negative direction until a limit switch is encountered. After all axes have reached limit switches the position counters are reset to zero. **Move to …** allows the user to instruct the positioning system to move to any location. **Set method** is used to select the number of samples, axis, and distance between samples for a measurement scan. **Go to start** instructs the positioning system to move to the starting point of a scan. **Scan X-section** instructs the positioning system and the Accumet™ meter to take samples along a path as defined by the method. **Save graph data** prompts the user for a file location and name and then saves the acquired conductivity data to disk. **Quit** exits the VI.

Evaluation

The new laboratory course was offered for the first time in the fall of 1995. Because the undergraduate laboratory course is completely new we are unable to make a true comparison with a non-computerized laboratory. However, we also offer graduate level laboratory courses that began using the Virtual Instruments and thus we can make the following observations.

The use of VIs helped make it possible to develop a state of the art laboratory from basic concept to full implementation in approximately 1.5 years.

Students were able to quickly learn how to use new instruments with capabilities designed to meet the specific needs of an Environmental Engineering laboratory and only a small amount of class time was spent explaining how to use the Virtual Instruments.

Automated sampling made it possible to collect high quality data for analysis of time varying processes (acidification of lakes, oxygen sag in rivers, pollutant mixing in rivers, and dispersion in reactors).

Students were able to analyze samples efficiently even when the instruments were operating in a manual mode (i.e. titrations and individual sample analysis on the spectrophotometer and gas chromatograph).

The ability to customize the Virtual Instruments to perform specific analyses adds great flexibility and will make it possible to continue to improve the laboratory experiments.

Availability of software

It is the intention of the authors to make the VIs described in this paper available to other educational institutions through the world wide web in the near future. In the interim, requests for code or assistance will be addressed to the best extent that time permits. Dr. Weber-Shirk can be contacted through e-mail at MW24@cornell.edu to obtain information on the availability and specifications of the software.

References

MONROE L. WEBER-SHIRK is an instructor at Cornell University in the School of Civil and Environmental Engineering. He teaches courses in environmental engineering and in hydraulic engineering. He creates software for instrument control and data acquisition for research and teaching applications. His research is on particle transport and attachment to surfaces in engineered and natural systems.

LEONARD W. LION is a Professor at Cornell University in the School of Civil and Environmental Engineering. He teaches graduate classes in water chemistry and physical/chemical processes and an introductory environmental engineering class. His research relates to the integration of chemical and biologically mediated reactions that influence contaminant fate and transport.