# Computer Simulation of Electronic Circuits Used in Chemical Instrumentation

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# Computer Simulation of Electronic Circuits Used in Chemical Instrumentation

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Most instruments used in modern chemical analysis contain specialized integrated circuits, transducers, detectors, and digital microcomputers. These devices control the operation of the instruments and often provide data manipulation capabilities such as Fourier transform, numerical integration and differentiation, curve fitting, and standardization. Major improvements in scientific instrumentation have resulted from the use of computers, as well as specialized integrated circuits. These call for an understanding of basic electronic circuitry at the undergraduate chemistry level. Although it is not necessary to study the individual components of chemical instrumentation in detail, a basic understanding of integrated circuits and data acquisition hardware will provide a conceptually straightforward, top-down approach to the implementation of electronics and computer technology (*1, 2*).

Current texts include such topics as electronic components, circuits, operational amplifiers, digital electronics, microprocessors, signals, and noise (*1, 3–5*), and several workers have incorporated computers and electronics into undergraduate chemistry curriculum. For example, Scheeline and Mork reported the use of computers to teach electronics to science majors (*6*); Hargis and Evilia described a semester-long course on electronics, interfacing, and online techniques for scientists (*7*); Braun presented laboratory experiments involving operational amplifiers and other electronic circuits (*8, 9*); and Wohltjen et al. described an instrument simulator capable of generating analog signals, which are equivalent to the analog outputs of most instruments (*10*).

Despite all these efforts, problems remain in achieving the goal of incorporating basic electronics into undergraduate curricula. First, the conventional approaches of teaching electronics in chemical instrumentation emphasize either the use of computers or hands-on experiments involving macroelectronics. Second, few if any of these approaches provide the connection between the basic electronic theories and their relationships to chemical instrumentation. Third, there is the issue of what to remove from current curricula. A typical instrumental analysis course focuses on the understanding of the fundamental principles behind the operation of chemical instrumentation. Therefore insufficient time is devoted to the electronic aspects of instruments in general. Finally, depending on the class size, the time and cost associated with acquiring necessary personnel and equipment could pose a limitation, especially in departments with modest means. Consequently, most chemistry departments have a curricular component that deals with electronics in instrumental and physical chemistry courses. Some schools teach basic electronics in engineering and physics classes. Although much of basic electronics is covered in these courses, the material is not usually presented in a format intended for chemistry majors who are taking an instrumentation course.

Here we present computer-aided design of integrated circuits and hands-on laboratory experiments that will give students practical experience in basic electronic circuitry. The experiments are based on the premise that information technology can assist certain conventional learning and teaching environments (*11–13*). In addition, computer-aided course delivery is cost effective, allowing students to run virtual experiments and quickly make changes to experimental parameters while instantly viewing the desired results. (These are not, however, intended to replace actual real-life applications.)

At SUNY-Binghamton, we have successfully used a computer simulation program known as Electronic Workbench (EWB) as part of our undergraduate laboratory curriculum. EWB is a user-friendly program that simulates electrical and electronic circuits. In the first part of these exercises, students were introduced to basic electronic concepts using Ohm's law, Kirchoff's rule, and theorems using computers to visualize these relationships. Next, the program was used to "design", simulate, and analyze simple dc and ac circuits. Results of these simulations were compared with actual experimental implementation and their relationship to chemical instrumentation was examined.

## Materials

Electronic Workbench software simulator (Interactive Image Technologies Ltd., Ontario) comprises SPICE (Simulation Program with Integrated Circuit Emphasis) and the SPICE Code Model Subsystem. Other materials used are PCs, solderless breadboards, resistors, resistance substitution boxes, capacitors, binary counters, analog-to-digital converters (National Instruments), 25-kW potentiometers, multimeters, cables, and power supply.

## Theory

Relevant lecture topics were covered before the exercises were attempted. Topics included Ohm's law, Kirchoff's rules, Thevenim's theorem, and amplifier circuits and applications and their properties, advantages, and limitations (*14, 15*). The laws and theorem were used to introduce these important circuit theories.

### *Definitions and Theorems*

*Voltage.* The voltage between any two points in a circuit is equal to the algebraic sum of the voltages produced by each voltage source separately.

*Current.* The current passing through any point in a circuit is the algebraic sum of the currents due to each current source in the circuit.

*Thevenin's Theorem*. A real voltage source in a circuit can always be replaced by an ideal voltage source in series with a generalized resistance. An ideal voltage source is one that can maintain a constant voltage across its terminals regardless of load (i.e., it has a zero internal resistance).

### *Current–Voltage Relations*

Ohm's law is the most valuable relationship for interpreting electronic circuits. For dc and ac circuits, Ohm's law can be used to quantitatively relate current, voltage, and resistance. The relationships for voltage ($V$), current ($I$), resistance ($R$), capacitance ($C$), and inductance ($L$) are as follows:

$$V = IR \tag{1}$$

$$V = \frac{1}{C}\int I \, \mathrm{d}t \tag{2}$$

$$V = L\frac{\mathrm{d}I}{\mathrm{d}t} \tag{3}$$

where $R$ is measured in ohms, $C$ in farads, and $L$ in henrys.

### *Loops and Nodes (Kirchoff's Voltage Laws)*

Most circuits contain a network of resistors, capacitors, or inductors within at least one branch. In this case, before Ohm's law can be applied, the circuit must go through a systematic reduction of the network. Kirchoff's law helps to solve circuit problems where resistors are interconnected to form a network. The law states that the sum of the rises and falls of a potential (or voltage) around any closed path is zero:

$$\sum_i V_i = 0 \tag{4}$$

It therefore follows that the voltage and current laws are a consequence of the conservation of energy and charge, respectively.

## Procedures

### *Part 1: Introduction to Electronic Workbench and Computer-Aided Design of Circuit Components*

This section introduces students to EWB and familiarizes them with the building blocks of electronic circuits, including resistors and capacitors. Frequently measured parameters in chemical instrumentation include voltage, current, resistance, charge, and capacitance. These parameters can be simulated and their values calculated using virtual experiments to understand how most electronic circuits work. This section also serves as a prerequisite to the study of operational amplifiers. It teaches students the characteristics of voltage dividers and series combinations of resistors and capacitors. The first step is to learn how to use EWB software and then apply the knowledge gained in assembling simple analog circuits.

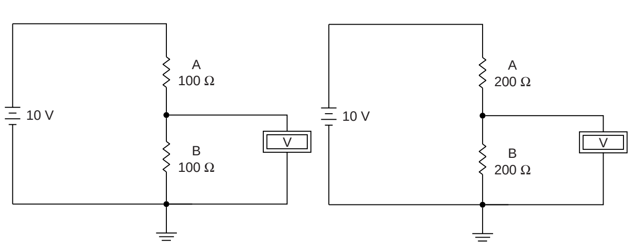


Figure 1. Design of analog circuits in series with a voltage divider using two (left) 100-Ω and (right) 200-Ω resistors. The voltage readings are the same, illustrating Ohm's law.

### Student Activities and Learning Experiences

To run this program, install EWB software and then find the EWB executable file from the Start menu and follow the steps outlined below.

1. First familiarize yourself with all circuit symbols for various electronic components: battery, operational amplifiers, resistors, capacitors, etc.
2. To build a circuit, assemble the required components by clicking the *Parts Bin Toolbar* and dragging these circuit components onto the circuit window, thereby creating a Component library for the circuit.
3. Rotate the resistors into vertical positions by double clicking and then choosing *Circuit/Rotate* on the Toolbar.
4. Wire the assembled components together by dragging a wire from the terminal of one component to the terminal of another component as required.
5. You can change the parameters of a component (e.g. resistor's resistance, a battery's voltage) by double clicking the component and making changes in the corresponding menus.
6. To test the voltage or current generated from the circuit, attach a voltmeter to the circuit by dragging the voltmeter from the Indicator's toolbar to the circuit window and position it to the right of the circuit.
7. Activate the circuit by clicking the power switch at the top right corner of the EWB window. NOTE: If the circuit is properly built, the voltmeter should display numbers that are consistent with the expected values based on calculations. If not, you will need to correct the errors and test the circuit again until the expected calculated values are obtained.

*Example.* The simple analog circuit shown in Figure 1 (left) consists of a ground, a 10-V battery, two 100-Ω resistors, and a potentiometer connected in series and two resistors acting as voltage divider. Place these components into the circuit window and arrange them in such a way that the resistors can rotate, so that they can be wired neatly into the circuit. Each component has a preset value that can be changed for specific needs. After construction, test the circuit by attaching a voltmeter from the Indicator toolbars. Activate the circuit by following Step 7 above. If everything is correct the voltmeter should now read 5.00 V, since two resistors of the same resistance divide the voltage from the battery in half. If the voltmeter does not read 5.00 V, check the values of the battery and resistors and make sure the circuit is wired properly. In addition, check that the voltmeter value is set to 1 MΩ under dc mode. By changing the resistances to 150 and 200 Ω and activating the circuit again, additional voltage readings can be taken. The analog signal output can be calculated by applying Ohm's law and Kirchoff's voltage law described in eqs 1–4. Since the resistors had a 1:1 ratio, each resistor will receive half of the voltage input. Therefore, the voltmeter should remain at 5.00 V after both resistors are changed to 150 and 200 Ω (Fig. 1, right). Students are reminded that resistors are among the most important components of electronic circuits and are commonly used as voltage dividers and potentiometers. In addition, resistors can be used with capacitors to provide a wide range of frequency-sensitive devices such as filters found in absorption spectrophotometry.

*RC Circuits*. After students have gained familiarity with the EWB software, they can then learn how to simulate the behavior of an actual circuit. For this exercise, a simple circuit to be considered is a series RC (resistive and capacitive) charging circuit. An RC circuit can be constructed using the following materials connected in series with a ground, a 10-V battery, a 20-mF capacitor, a 10-kΩ resistor, and an oscilloscope with a ground as shown in Figure 2. The circuit configuration can be saved on file for further manipulation. An oscilloscope is one of the test instruments that can be used to analyze analog circuits. The simulated oscilloscope is a dual-channeled digital scope instrument capable of displaying waveforms of one or two electronic signals so that the magnitude and frequency can be analyzed over a period of time.

The oscilloscope is connected to the RC circuit built from an earlier exercise by simply clicking the oscilloscope icon on the Instrument toolbar. A terminal on the oscilloscope icon is then highlighted and the wire is dragged to connector "A" in the circuit. If the other terminal is highlighted on the oscilloscope icon, a wire can be dragged to connector "B". Finally, the circuit window is connected to ground. The controls of the oscilloscope can be adjusted by double-clicking on its icon and setting the time base in the oscilloscope precisely according to horizontal divisions per second.

In this exercise, the oscilloscope was set at 0.1 s/div and the circuit was activated. When a signal is first applied to a real circuit, there is a transient response before the circuit settles down to its usual steady state. After a few seconds, students can activate the circuit and observe the output-charging curve. If the charging curve is unnoticeable, the settings on the oscilloscope should be checked to ensure that all wires are properly connected and the ground terminal is in place. The charging curve demonstrates the RC time constant formula, in which one RC time constant (TC or τ) is equal to R (in ohms) times C (in farads). In this case TC = 10 kΩ × 20 µF = 0.2 s. Approximately 5 time constants are needed to fully charge the capacitor. Using the same assembly, students can vary the time base to 0.2, 0.5, and 1.0 s/div and the oscilloscope will automatically redraw the waveforms.

### *Part 2: Computer Simulation of Operational Amplifiers and Implementation on Solderless Breadboard*

This section is designed to acquaint students with the basic principles of operation of integrated circuits, with focus on operational amplifiers (op-amps). Op-amps are widely used in modern chemical instrumentation for precise measurement of voltage, current, and resistance. They are also used to perform mathematical operations such as addition, multiplication, integration, and differentiation. Students can work on two closely related activities such as the use of EWB to design and test a number of op-amp circuits, or the actual construction of the circuits with op-amps using solderless breadboards.

### Student Activities and Learning Experiences

This exercise can be used to teach the general characteristics of op-amps and the associated symbols and properties. It is possible to design circuits that provide nearly error-free amplification, effective processing of signals (e.g., filtering, differentiation, attenuation), and precise and stable values of voltages and currents. Using EWB, students assemble the circuits shown in Figure 3 and input 5 or 6 voltage values (ranging from 0.0 to 1.2 V) using the variable voltage source attached to the inverting and non-inverting amplifiers. They record the corresponding output voltage for each input and answer the following questions. Did the output give the expected results? What expressions give the input voltages in terms of the output voltages and resistances for the circuits in Figures 3b and 3c? In Figure 3b, what is the output volt-

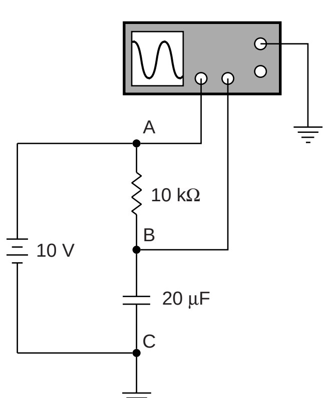


Figure 2. Design of RC circuit using computer simulation. Circuit was constructed using a 10-kΩ resistor and a 20-µF capacitor in series and a voltage source of 10 V.

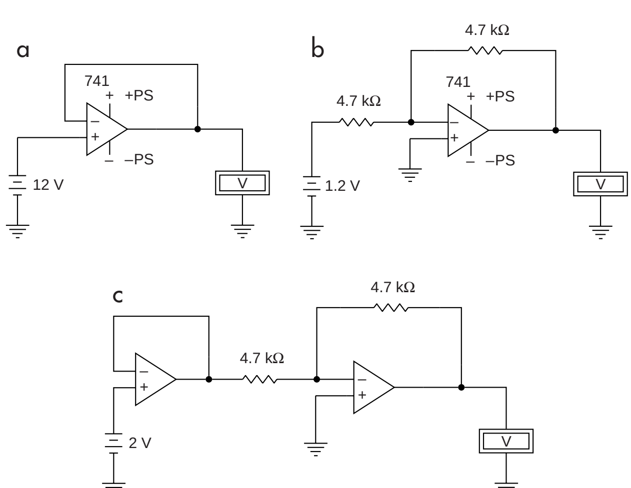


Figure 3. Examples of operational amplifiers used in chemical instrumentation: (a) voltage follower, (b) inverting amplifier, (c) high-impedance potential measuring device.

age when the input voltage is at the non-inverting position? Comment on the linearity of the output vs input voltage. What is the main advantage of using the device in Figure 3c over the one in Figure 3a for potential measurement?

*Building Circuits on Solderless Breadboards.* In this exercise, students learn how to construct circuits with operational amplifiers using a solderless breadboard. The hands-on experience of making electrical connections differs from simulation in that instead of dragging the wires on the screen, students actually build the circuit on the breadboard. The solderless breadboard consists of a spring-loaded connection to wires running in different directions. It requires no soldering, so students cannot be burned. The standard way of making an electrical connection is to use a piece of wire with no connectors on either end. The power supply is mounted on the right side of the breadboard using +12 V, −12 V, +5 V, and ground sources. The three devices in Figure 3 are built from wire connections, resistors, and operational amplifiers. Braun et al. have described experiments dealing with the use of op-amps in instrumental analysis (*8*), and readers are advised to consult this paper for details of pin assignments of the LM 741 op-amps. In this exercise, at least two sets of input values are obtained for each device and the corresponding output values are recorded. These are then compared with expected results based on calculations and simulation.

### *Part 3: Application of Electronic Circuits Studied to Chemical Instrumentation*

Applications of electronics in chemical instrumentation and design are of interest to chemists in several areas. Examples are the accurate measurement of current in voltammetry, coulometry, photometry, and in ionization detectors in chromatography. The methods described in this paper can be adapted to teach students several operations central to chemical instrumentation. Demonstrations include the application of op-amps to the measurement of a small photocurrent.

### Student Activities and Learning Experiences

The goal is to design a low-resistance current-measuring device. This is achieved by removing the resistor $R_i$ in Figure 3b and using the current to be measured as the signal input. The resulting device is shown in Figure 4. In the laboratory, this device can be used to measure the absorption of light by a colored analyte placed between the light source and the solution. The resulting voltage is then related to the concentration of the species in the sample that is responsible for absorption following Beer's law. A small dc current is generated by a photomultiplier tube (PMT), which converts the light into an electrical current. If the cathode of the PMT is maintained at a negative potential relative to the anode, absorption of radiation by its surface results in the ejection of electrons. These electrons are accelerated to the anode and a small current ($I_x$) is produced that is directly proportional to the power of the radiant beam. The circuit also provides compensation of PMT dark current. The output potential ($V_0$) corresponds to the potential difference across the resistor $R_f$. From Ohm's law,

$$V_0 = -I_f R_f = -I_x R_f$$
$$I_x = \frac{-V_0}{R_f} = kV_0 \tag{5}$$

Hence the potential $V_0$ measured gives the current, provided $R_f$ is known. Students can experiment by changing the $R_f$ values from 50 to 500 kΩ, measuring the potential generated at the meter, and calculating the small current from Ohm's law.

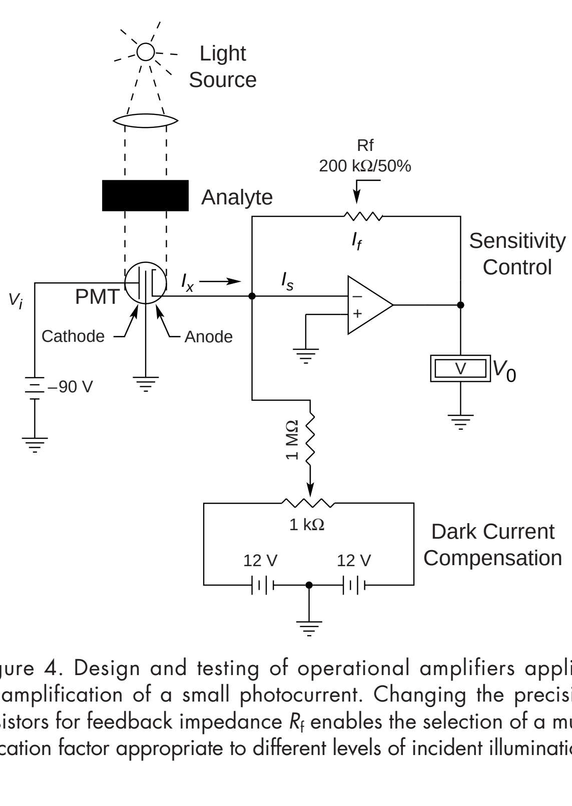


Figure 4. Design and testing of operational amplifiers applied to amplification of a small photocurrent. Changing the precision resistors for feedback impedance $R_f$ enables the selection of a multiplication factor appropriate to different levels of incident illumination.

## Supplementary Materials for Students and Instructors

This paper provides background information on the use of simulation software and the implementation on a solderless breadboard. The information provided should be sufficient to enable anyone with a little background in building electronic circuits to repeat the experiments, which can be completed in two laboratory sessions. The materials assume some familiarity with the basic theory of electronics that should be covered during lecture before the laboratory exercises. Additional information can be obtained from Web sites devoted to using EWB software (*16*). Although we chose EWB, there are several other computer software packages that also enhance electronic design processes. Of these, SPICE is by far the most widely used. This program was developed at the University of California, Berkeley, in the mid-1970s. The software has since become public domain and versions of SPICE exist on computers and workstations at universities, companies, and institutions worldwide.

Instructors may include other pertinent experiments on chemical instrumentation such as the design of a simple potentiostat. A potentiostat is an electronic device that maintains the potential of a working electrode at a constant value relative to the reference electrode. A device might be constructed for use with a three-electrode electrochemical cell such as the one shown in Figure 5. The aim is to keep the potential difference between the working electrode and the reference electrode constant. Since the voltage at the reference

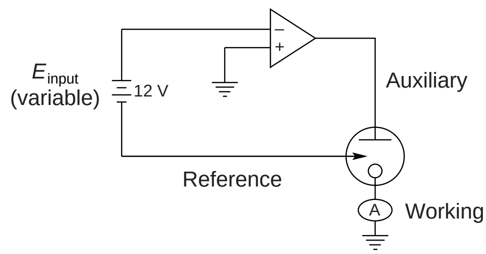


Figure 5. Design and testing of a three-electrode potentiostat. When a potential is applied to the working electrode, a low current is measured regardless of the changing resistance or concentration polarization of the solution.

electrode is fixed and the working electrode is at ground potential, the potential at the follower input is $E_{ref}$. When $E_{input}$ is added to $E_{ref}$, the amplifier generates a potential of the opposite sign at the output. Through the use of Ohm's law, the value of $E_{ref} - E_{working}$ can be deduced. The major differences between a computer-aided circuit cell design and one with real solution components should be pointed out to students: (i) the feedback $R_f$ is now the solution resistance between a pair of electrodes, and (ii) the circuit consists of a booster amplifier, a standard noninverting amplifier that permits a much larger current than can be furnished by most op-amps. Other suggested experiments may include how filtering is achieved in spectroscopy or how amplifications in transistor circuits are developed and modulated.

## Summary

Computer simulation is used to illustrate the fundamentals of electronics and electrical circuits as related to undergraduate chemistry laboratories. Results are correlated with experimental data obtained from breadboard experiments. The basic components of electrical circuits, including resistors, capacitors, inductors, potentiometers, and oscilloscopes are introduced. Analog circuits are designed and analyzed and results are compared with laboratory-generated measurements. Simulation reinforces the underlying principles of electronics as used in chemical instrumentation. The experiments can easily be modified for the design and analysis of other chemical instrumentation, including construction of a portable potentiostat/galvanostat and building of a sensor-switching device. The experiments provide a good introduction and effective exercises for undergraduate chemistry students by applying electronic theories to the operation of chemical instrumentation.

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