

Virtual Chemistry Laboratory for Non-Science Majors, Good or Bad?

By

John H. MacMillan Ph.D.



Chemistry educators can become overly mesmerized with the potential for computerized instruction in the science laboratory, particularly chemistry lab.

Radical advocates could go as far as introducing a total software based laboratory, with all laboratory manipulations and data collections virtualized on the computer screen. Lab software is now available allowing this approach.

At both the high school level and college level for non-science majors the following arguments could be made for an exclusively software based laboratory.

- a) The students gain computer literacy as they learn the logical methods of analysis and synthesis practiced in the laboratory.**

- b) The students can generate, analyze and graph data very quickly.**

- c) **More difficult experiments involving hazardous manipulations or toxic chemicals can be performed in the virtual laboratory.**
- d) **Potential for student injury is minimal. Lawsuits from such injuries are eliminated.**
- e) **Handicapped students can perform the experiments more easily.**
- f) **Toxic waste disposal costs are minimized.**

At the college level all the above factors also apply. In addition at large universities there are hundreds of students in allied health, medical technology and other fields where arguments could be made for a totally virtual laboratory. These students work at the technician level and are trained in whatever techniques are necessary at their employers. Pre-meds and science majors of course must be exposed to glassware and instrumentation at the college level. Minimized waste disposal costs are a compelling factor at large universities. To logically analyze the issue we must try to answer three questions.

- 1) What is the role of the computer in science?**
- 2) Are we educators, educational businessmen or bureaucrats?**
- 3) Would the students learn more scientific methodology with totally computerized laboratory?**

Scientific and technical people tend to be fascinated with computer technology. This author has seen several colleagues who have become so

immersed in the computer that they perform very little laboratory work! To answer question one we must remember that in experimental science the computer is a tool and not an end in itself. It is this author's view that any laboratory program that is exclusively computer based presents a distorted view of science to the student. Experimental science is intrinsically hands-on. Part of the scientific process is learning to manipulate equipment, work with real chemicals, and interpret real physical phenomena.

Question two poses a problem to the educator of conflicting priorities. The teacher may be under pressure from the principal or department head to minimize costs and potential legal liabilities. Virtual laboratories can be a pleasing "cop out" for administrators or bureaucrats whose concerns are not purely educational. The teacher can be put in a compromising position if he sits on financial committees. Each educator must balance his priorities as best he can in his unique situation but in all instances educational integrity and student progress must take priority. Many educators argue in response to question three that virtual laboratory would be more thorough and introduce the students to a far greater range of experiments and laboratory manipulations than conventional laboratory. This author counters the argument by first conceding that more "experiments" are indeed possible but these virtual experiments are distorted from the real scientific method and thus are of diminished educational value. A minimalist approach where a fewer number of experiments are done manually can be of greater value if chosen carefully. We will elaborate on these issues in greater detail below.

There is an abundance of software for science and other education but a paucity of studies on the effectiveness of the instruction. In light of this situation,

this author is somewhat conservative in implementing radically new programs. I give as anecdotal evidence for caution my experience at a large urban university with "micro-laboratory" for organic chemistry. In this approach the students are hands-on but all experiments are in micro glassware on 50-100 milligram scales. This laboratory is given for all premed and science majors in the sophomore year. The theoretical educational and financial advantages of this approach are:

- 1) The students must develop neat and precise working habits to work with the small quantities of materials.**
- 2) Potential for injury due to explosion or fire is minimized.**
- 3) Costs of waste disposal are radically reduced.**
- 4) Glassware breakage is drastically reduced.**

I entered this laboratory enthusiastically, fully expecting to find the approach educationally sound and fun for the students. After the novelty of the micro training and first weeks wore off, however, problems with the approach became evident. Among them:

- a) At this scale the students could not readily see the exotherms, color changes or precipitation's that are an integral part of organic synthesis. All experiments looked alike!**
- b) Achieving high percentage yields was nearly impossible at this scale. The students became increasingly more frustrated as the weeks progressed.**

c) The instructor could not readily grade the quality of the products produced, since the small quantities obtained were consumed in spectral and chromatographic analysis.

d) This author is aware of true industrial synthetic scales. Except for some Pharmaceutical and Biomedical research, the vast majority of industrial synthesis is at a much greater scale, often from 500 grams to multi- kilogram quantities!

e) The students confided in me that they were "bored silly" by the sameness of the approach. When I described the old scale preps, which typically ran at 2-10 gram scale, they wistfully longed to be a part of the earlier program.

What went wrong here and how would I modify the program? Obviously cost containment had won out over educational value in this instance. This author tends to favor compromise approaches. Obviously good technique is taught by the micro synthetic approaches but only three or four experiments per semester should be devoted to them. Larger scale experiments must be introduced both to give students a more rounded view of real world chemical reactions and to hold their interest. If this approach means two sets of glassware and added chemical disposal costs, so be it! The faculty must confront administrative types when necessary and fight for sound laboratory programs.

While this author has no educational research data to reinforce the argument below, his strongly held views, based on over twenty years of teaching, are that the virtual laboratory can readily fall into a similar trap to the micro laboratory if it is

exclusively used or overused during the term. Problems similar to the micro laboratory are:

- a) The students gain a distorted view of real laboratory work and real chemistry. Here the problems can be even more acute than for the micro laboratory, since no real glassware manipulation or working with chemicals is involved.

- b) While most students are eager to work with the computer, a certain restlessness to actually work with their hands will doubtless surface over the term. Teacher demonstrations are not enough for most students. They enjoy the real color changes, manipulations and even odors of the chemistry, biology or general science laboratory.

Therefore this author again favors a compromise approach. Many hands-on experiments involving titration, kinetic studies, gas laws or thermodynamics can use the computer to enter, graph and search the data without making it the exclusive workstation.

Many experiments can use benign household substances such as vinegar or baking soda to minimize toxic waste and potential for student injury. Perhaps twice a semester, experiments generating or using toxic substances such as chlorine or nitric acid can be totally "virtualized." The students will both enjoy the variety and be more thoroughly educated in real scientific laboratory practice.

Science laboratory gives a different relative importance to these types of programs as compared to classroom instruction. In chemistry laboratory the spreadsheet is in this author's opinion the most useful program. Many experiments

lend themselves naturally to tabulation, computation and graphical analysis. Databases are the next most useful programs. Useful experiments involving a database often involve group analyses where an entire classroom data can be entered and trends discerned. Environmental studies such as acid rain or household chemicals neatly fit these programs. Also of use uniquely in chemistry laboratory are molecular modeling programs. These programs allow the student to construct, rotate, scale and compare individual molecules on the computer screen. One laboratory per semester should be given to such activities, but again I am against a totally virtual approach. The computer should be used in conjunction with hands-on conventional molecular modeling kits. In my opinion the students gain much insight in stereo chemical relationships and enjoy physically constructing the models from ball and stick kits. Molecular modeling programs are most useful in looking for "lock and key" effects when they are introduced to more complex molecules such as peptides or enzymes. Conventional word processors are of least utility in chemistry laboratory. While in principle the lab reports could be written on the word processor, this technique conflicts with real world laboratory practice. For patent protection all industrial and academic research laboratories employ hand written bound notebooks with spaces for signatures at the bottom.

The issue of handicapped students often is raised as a compelling reason for virtualized computer instruction. Indeed the computer does allow the physically disabled much greater latitude in performing their own work. I feel however that handicapped students should attempt to work at the same hands-on/virtualized experiment ratio as the other students; both for generating self-confidence and social skills the handicapped should attempt full laboratory integration. For difficult manipulations they can easily work with a partner. For computer-assisted laboratory they may be assigned the task of entering the data on the computer. The remainder of this paper will show instances where computer assisted laboratory

instruction may be of value without virtualizing the entire laboratory experience.

"Variety is the spice of life" especially in the experimental sciences. A totally virtual world is inappropriate in the sciences, since the real world we discover is so fascinating!

Below are several examples of computer based "dry" experiments to illustrate possibilities.

EXAMPLE 1

The kinetic data below are for the reaction of methyl iodide with sodium ethoxide in ethyl alcohol. The products of the reaction are methyl ethyl ether and sodium iodide.

T°C	k ₂ (liters/mole sec)
0	5.60(x 10 ⁻⁵)
6	11.8
12	24.5
18	48.8
24	100
30	208

REF.: W. Hecht and M. Conrad, Z. physik. Chem., 3: 450 (1889)

- Write the balanced chemical equation.
- Using a commercially available spreadsheet program such as EXCEL import the data, define all fields.
- Graph the data in the appropriate manner. You decide the proper graph type!
- Calculate: x-intercept, y-intercept, Arrhenius energy, "A" factor and entropy of activation.

e) Calculate the standard deviation and error limits for the above values.

Tabulate all data in the spreadsheet, print and pass in the work in three days.

Good luck!

EXAMPLE 2

HOMEWORK ASSIGNMENT

GAS DENSITIES, WILL A BALLOON RISE OR FALL?

We have learned in this chapter how to calculate gas densities from the Ideal Gas law. The density of a gas as compared to that of air is of great practical utility. Gases with a low relative density could in principle be used in blimps or in balloons so as to rise when released. Conversely, and perversely, gases of high density relative to air will "hang" close to the ground and do not dissipate easily. If toxic, such a gas could be used as a chemical warfare agent. Several such gases were actually used in World War 1. Your task is to:

1) Calculate the density of air at STP. Assume a composition of 80% nitrogen and 20% oxygen. Since this gas is dry while real air contains water vapor, the value will be slightly high, but will serve for this analysis.

2) Setup a spreadsheet that automatically calculates the density of any gas at "STP", standard temperature and pressure.

3) Calculate the densities of each gas below at STP. Tabulate the data in the spreadsheet.

4) Arrange the data in a table listing the lightest at the top. Place the value of air calculated in #1 above in the table.

5) List whether a balloon would rise or fall if filled with this gas.

6) Comment on the most effective gas for blimps. Is there a practical reason why this gas is not used?

7) Comment on which gases would be effective chemical warfare agents.

Why

were such gases not used in World War 11?

Your spreadsheet should have headings as below.

GAS, FORMULA, MOL.WEIGHT, DENSITY(g/cc), RISE or FALL? , COMMENTS

GASES

Ammonia	Hydrogen bromide	Nitrogen
Carbon dioxide	Hydrogen chloride	Nitrogen dioxide
Carbon monoxide	Hydrogen iodide	Nitrous oxide
Chlorine	Hydrogen cyanide	Oxygen
Helium	Hydrogen sulfide	Phosphine
Hydrogen	Nitric oxide	Phosgene

Graph the data in your spreadsheet using molecular weight and densities as the axes. Present the graph in two different formats. Print and hand in your spreadsheet.

EXAMPLE 3

ACID RAIN, CLASSROOM EXPERIMENT

For the next three months collect rain samples when there is precipitation in your area. Note where the sample was taken, the date, the temperature, whether rain or snow and whether collected from falling rain or taken from the ground. For all samples bring them to school the next day and measure the pH using the pH meter. Record all data above on the standard database on the laboratory computer. At the end of this period search the data and those of your classmates for specific pH ranges. See if you can deduce any correlation between pH and time of year, location or method of sampling. Present your data in spreadsheet format and write a two-page report on your findings.

EXAMPLE 4

DEDUCING OPTICAL ISOMERS USING BOTH PHYSICAL MODELS AND A MOLECULAR MODELING PROGRAM SUCH AS "SPARTAN"

Make ball and stick and computer generated molecules for the compounds below. Deduce if optical isomers are possible and the number possible. For those capable of optical isomerism generate both enantiomers on the computer screen and rotate them to a "mirror image" relationship. Save the files for the mirror images. Tabulate your data in a spreadsheet program and import the mirror image structures into your spreadsheet. Print your results and hand in the assignment in three days. Have fun!

COMPOUNDS

CHLOROMETHANE

BROMOCHLOROMETHANE

BROMOCHLOROIODOMETHANE

BROMOCHLOROFLUOROIODOMETHANE

1,2-DICHLOROETHANE

1,1-DICHLOROETHANE