

## Discovery-based General Chemistry Using Chemland Simulations

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### Introduction

This paper describes a set of simulation programs for discovery learning in general chemistry and offers commentary on their use for enhancing the learning experience for introductory chemistry students. In traditionally taught general chemistry classes, students are taught the basic concepts of chemistry. This is normally done in the lecture portion of the course, and may involve various degrees of active learning strategies. These courses also teach how experiments are used to obtain scientific data by having students perform experiments in the laboratory section of the course.<sup>1-3</sup> In recent years these laboratory experiences have often become more investigative, allowing students to design experiments to answer specific questions.<sup>4-14</sup>

These two parts of a course represent the two ends of the continuum of the scientific enterprise. We teach how to obtain data and we teach general concepts. However, we do not often teach how large sets of experimental data are used by scientists to arrive at the conclusions we present, as given, in lecture. We often explain to students what chemists think, but not how they come to accept the science's accepted concepts. Students rarely get the opportunity to analyze data and infer broader principles from trends they may see in those data. In short, they do not fully have the opportunity to act as scientists. This is not surprising in that a single concept covered in lecture might represent years of careful experimental work. While the laboratory component of general chemistry addresses some of these issues, the scope of the laboratory work is very limited by time, ability, and cost. It is very difficult to generate enough data in the laboratory to allow discovery of concepts taught in the lecture. Even presenting all the data taken by an entire laboratory class together is seldom sufficient to allow one to discern the chemical or physical relationship governing the experiment performed. Discovery laboratories do allow the introduction of these concepts, but not their in-depth exploration.

Students rarely have the chance to ask "what if?" and to test their question. In recent years a number of educators have made use of computer-based simulations to allow student exploration to supplement either their lecture or laboratory work.<sup>15-23</sup> The Chemland modules described here serve to bridge the gap between what is possible in the laboratory and the concepts taught in the lecture. We see an opportunity to enhance the student's learning experience by using simulation software designed specifically to foster analysis of significant sets of data with the goal of developing their own understanding of chemical relationships from the data provided. Our goal is to guide students to discover for themselves the concepts taught in the general chemistry course.

### The Chemland Software Set

Chemland, a suite of freely available (<http://soulcatcher.chem.umass.edu>) exploratory general chemistry educational computer programs, has been written to augment standard book and lecture course material for introductory level chemistry with discovery-based learning exercises. Many of the modules are also available as Java applets, and can be found at <http://owl.chem.umass.edu/Chemland/chemland.html> (be sure to include the capital C).

Chemland consists of 64 interactive program modules written in Visual Basic. Figure 1 shows the main menu with the nine categories into which the modules are divided.

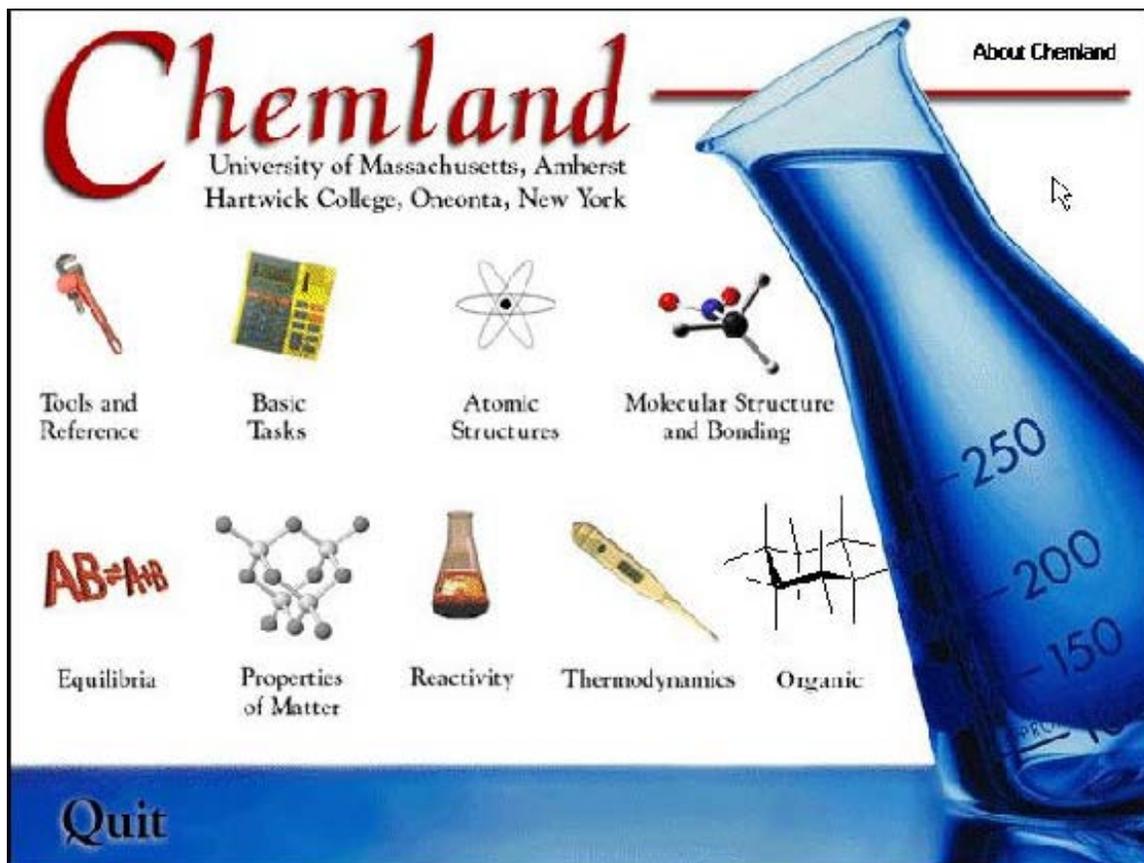


Figure 1. The Chemland Main Menu. Selection of each topic brings the user to a lower level menu screen containing links to modules for that topic.

◆ From each category screen, a selection of three to eight individual modules can be accessed. A chart containing all the categories and modules is shown in Table 1.

Table 1.

### Tools and Reference

Plotter  
 Preiodic Table  
 Unites of Concentration  
 Molecular Weight & Weight Percent

### Thermodynamics

Specific Heat  
 Calorimetry  
 Bond Energy-Heats of Reaction  
 Gibb's Law of Thermodynamics  
 Hess's Law  
 Heat Transfer

### Atomic Structure

Mass Spectroscopy

### Basic Tasks

Solution Making  
 Balancing Equations  
 Significant Figures  
 Ionic Compounds  
 Oxidation Numbers  
 Molarity Calculations  
 Dimensional Analysis  
 Elemental Analysis

### Properties of Matter

Gas Laws

Atomic Absorption and Emission  
Electromagnetic Spectrum  
The Photoelectric Effect  
Orbital Shapes  
Quantum Numbers  
Orbital Energies  
Electron Configurations

## Molecular Structure and Bonding

Coulomb's Law  
Molecular Polarity  
Bond Length/Energy  
Transition Metal Bonding  
UV-VIS Spectroscopy  
Metallic Bonding

## Reactivity

Limiting Reagents  
Rate Measurement  
Rates of Reaction  
Radioactive Decay  
Electrochemical Cell  
Net Ionic Equations  
Electrolysis  
pH of Salts



Operation of the free-standing modules has been verified on a large variety of hardware platforms running Windows95, Windows 98, and WindowsNT versions 3.5 and 4.0. The applet versions work on both Windows and MAC platforms, with the most consistent browser being Internet Explorer.

Various controls are assembled on the screen, allowing the user to get feedback based on offered input parameters. As a first example, the Electronic Configuration module is shown in Figure 2.

Henry's Law  
Gas Phase Boltzmann Distribution  
Liquid Phase Boltzmann Distribution  
Equilibrium Vapor Pressure  
Phases of the Elements  
Enthalpy of Dissolution  
Colligative Properties  
Real and Ideal Gases  
Density of Gases

## Equilibria

Chemical Equilibrium  
Acids and Bases  
Buffer Ph  
pH Titration  
pH Buffer Solutions  
Le Chatelier's Principle

## Organic

pH of Organic Molecules  
Boiling Point  
Heats of Hydrogenation  
Conformational Analysis  
Markovnikov's Rule  
Huckels' Rule

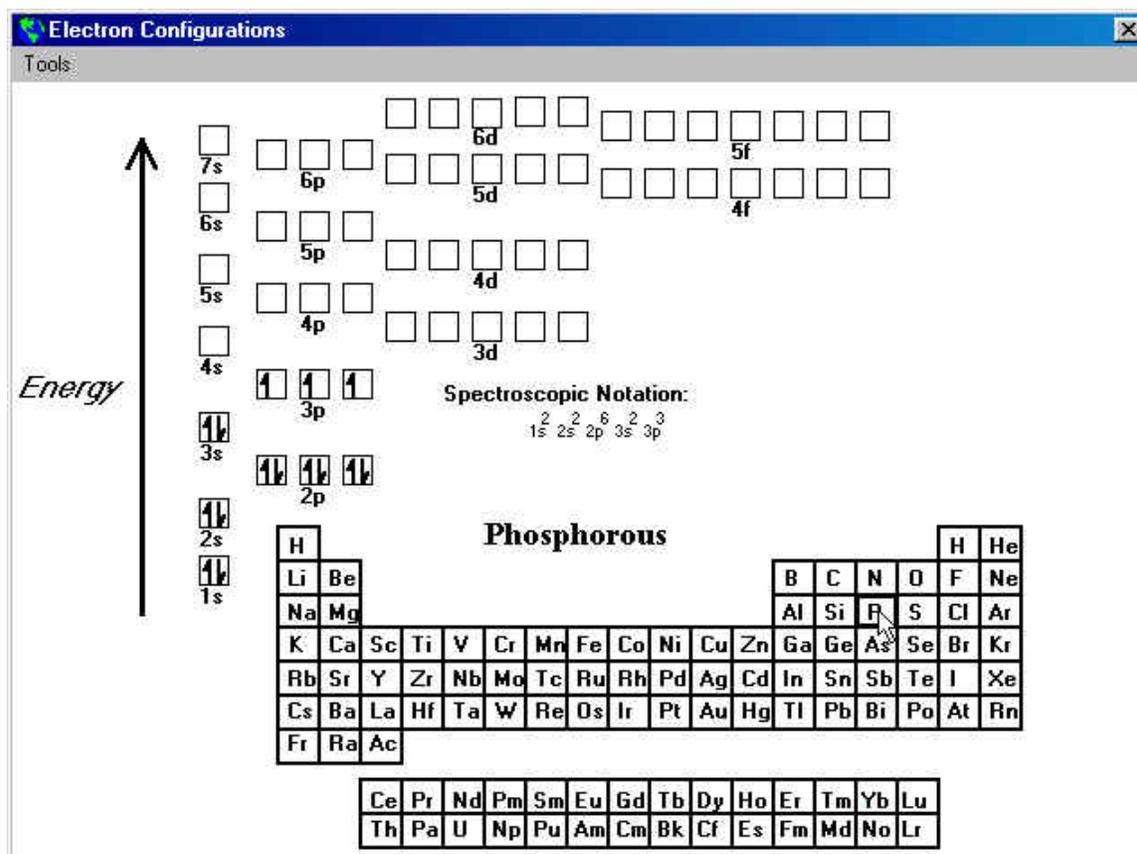


Figure 2. The Simulation Screen for Electron Configurations Simulation Module. The element symbol for Phosphorus has been selected.

For input, the user selects an element from the periodic table. The feedback returned is not in the form of laboratory measurements, but rather as the experimentally determined ground state electron configuration. This is given in two ways, both pictorially in the qualitative energy level diagram and in spectroscopic notation. ♦ An instructor could, for instance, use this module to state the Pauli antisymmetry principle in appropriate form and Hund's rule, and then connect the result of applying them to each element's position in the periodic table. ♦ As we use it, students explore the module for some length of time and discover those rules on their own. In our experience, students can use this module to teach themselves the rules for assigning electron configurations within about 15 minutes. We then spend the majority of class time discussing the reasons behind the rules they develop from the simulation.

As a second example, the Equilibrium Vapor Pressure module is shown in Figure 3.

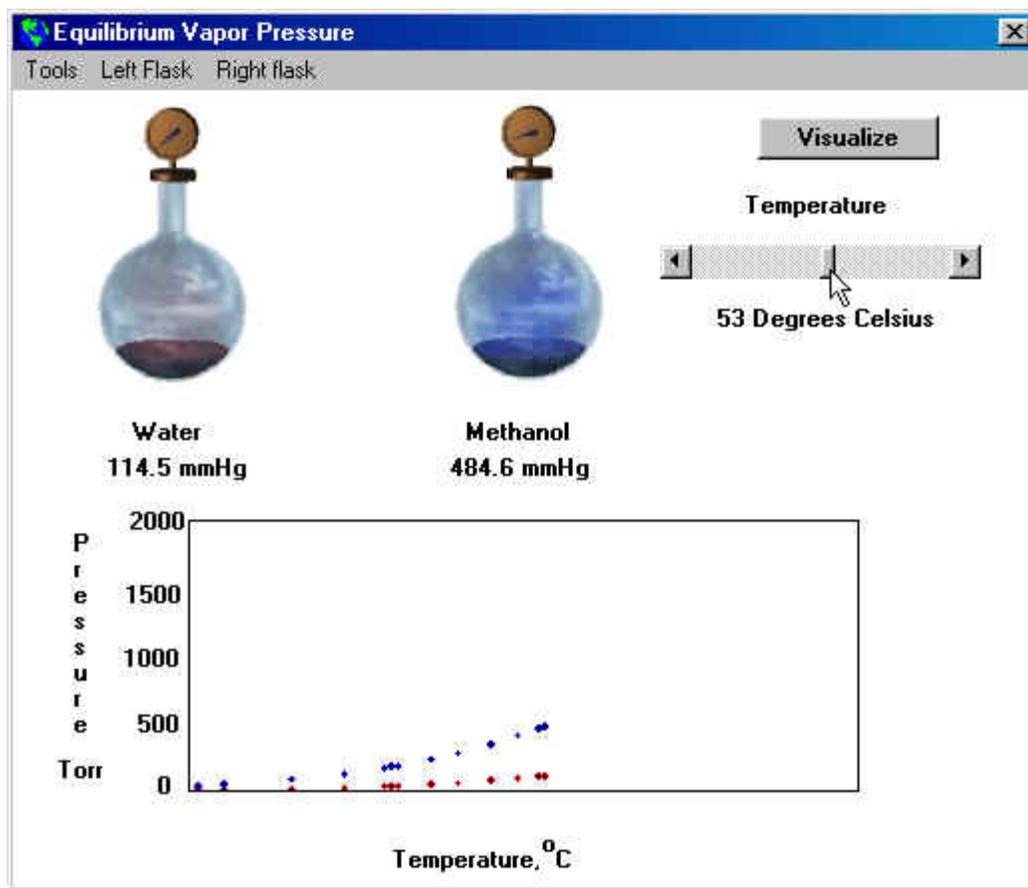


Figure 3. The Simulation Screen for the Equilibrium Vapor Pressure simulation module. The user has just adjusted the temperature to 53 °C.

This module simulates a series of vapor pressure measurements. This is an experiment that could be performed in lab with adequate equipment and time. The complexity of its correct execution is appropriate for a junior level physical chemistry course, yet the results are clearly of interest at the general chemistry level. The simulation allows selection of two liquids to study from a list of five, and variation of the temperature. Students can use the simulation to explore boiling point, the relationship between temperature and vapor pressure, and effects on these of molecular structure. The data obtained can also be used to calculate the enthalpy of vaporization for each liquid. In order to cater to different learning styles, we have also attempted to give an indication of change during the simulation in a variety of ways. In this case, the change in vapor pressure is seen numerically, graphically, as a darkening of the vapor part of the flask, and as a movement on the meters attached to the flasks.

## Development History

Chemland has been in use as an integral part of the general chemistry programs at the schools where it has been developed--Hartwick College in Oneonta, NY and the University of Massachusetts at Amherst--for six and three years respectively. The project began in the Summer of 1994, when Hartwick College initiated a program whereby each incoming first-year student would be given a laptop computer they could bring to class. We decided to create a set of simulation programs that could be used by students in class. The first version contained 24 program modules and was received very positively by the first students to use it. Since then, more modules have been added each year and we currently have modules covering most basic concepts taught in general chemistry.

We have chosen Visual Basic as our programming language for Chemland. Most of the modules have been programmed by undergraduate students, and Visual Basic offers an easy to use interface for designing highly interactive modules. The same results can be obtained using C++, but we have found Visual Basic to be much easier

for students to master. We find most students can begin work on useful materials within 2-3 weeks of starting to learn the language. It is generally the case that we spend much more time worrying about how we want to teach something than how to get that idea to work within the programming environment.

## Philosophy and Methods of Use

The basic philosophy behind this work is that students will understand a principle better if they construct that principle on their own. This interactive software provides a way for students to learn to think like chemists, to gather data and derive theories from those data. Using the simulated data from Chemland, students can obtain a broad sample of results not available in the lab class, derive the chemical principles underlying those observations, and test those principles.

The individual modules within Chemland provide interactive simulations of various observable and unobservable phenomena at both the macroscopic and molecular levels, allowing the user to change experimental parameters and observe results. We have intentionally not tried to create simulations of laboratory equipment or to make tutorial programs that show students how to solve problems. Software of this type is available and can be very useful, but our intent here is to center on exploration and understanding of conceptual relationships. Each module is designed to allow students to explore and obtain information, but offers little in the way of explanation. Explanation and synthesis of the information obtained using the simulations is integrated into the method by which the instructor runs their course. This is intimately tied to effectively guiding the student through the simulations.

Over six years of using these simulations, we have found them to be useful only when students are effectively guided through their explorations. Simply giving students a simulation and asking them to explore most often leads to little understanding. We believe that first-year college students are not at a level of sophistication where they know how to limit variables, perform multiple, controlled studies, and put the results of each study together into a coherent whole. Indeed, showing by example how to proceed in an investigation using these simulations is one of the main points to their use: to show students how to design and interpret broad studies. We have examined and found evidence that their use has a positive effect in this regard.



These programs have been used as in-class exercises in both large and small lecture sections and as the foundation for out-of-class assignments. In this paper we center on use in the classroom, where each student or small group of students has a computer.

### In-Class Use

The Chemland software was originally designed to encourage learning through the thorough exploration of a particular chemical phenomenon or laboratory-type experiment during a class period. Concepts normally told to students can now, instead, be discovered by those students for themselves. The ideal method of use is one where the instructor uses a computer, the image from which is projected on a screen for the whole class, and each student or small group of students have computers they can use at their desks. This is the case at Hartwick College where students bring laptops to class, and at UMass, where the class is taught in a technology rich Chemical Engineering Alumni Classroom (which holds 50 students, who share 25 networked computers).

Because our hope is for students to construct their own understanding of chemical phenomena, we use the simulations at the beginning of a topic. Ideally, a class period consists of:

1. A short (5 minutes) introduction to a topic by the instructor, defining what we will be studying, how it relates to other aspects of the course, and why it matters.
2. An extensive exploration using the simulation where students are led to discover the relationships of interest. This can take from 5 to 30 minutes, depending on the complexity of the material.
3. A summation of the topic by the instructor.

About half the available class time is spent during the extensive investigation. This takes place in multiple iterations. First the instructor shows how the simulation works and asks the students to perform an initial, very simple study. The

intent of the first study is to make sure the students know how to use the simulation and understand the information it offers. Students give their thoughts on the question and a short discussion takes place. This process is repeated for more and more complex aspects of the material, after each of which the conclusions reached by the class as a whole are recorded. Virtually everything recorded during the class period comes from the students.

At the end of this exploration, the instructor takes time to summarize the material. This serves to allow introduction of correct chemical terminology and to offer a clean set of notes for the students. Our first attempts at teaching in this manner led to rather poor note taking by the students, and in fact this remains a drawback to this teaching method.

Over time we have gained the following wisdom in leading discovery, discussion-based classes:

- Do not ask yes-no questions to initiate discussion
- Give students time to talk to and teach one another
- Emphasize the step-by-step path of the discussion
- Do start the discussion with an ultimate question to be answered; instead approach the exploration in an apparently open-ended way
- Limit simulations to 2-3 variables, but give a large range to explore within those variables

## Evaluation

Our hope is that the use of computer-based simulations in class will increase student learning. A number of studies have been conducted evaluating the use of computer simulations on student learning.<sup>24-28</sup> The use of Chemland discovery modules is expected to help ground students in a firm understanding of concepts, and this should positively effect their problem solving skills. However, the modules are centrally designed to increase a student's ability to derive concepts from sets of data, and it is here that we expect the most obvious advances in student ability. Therefore, we have studied the use of Chemland modules in two ways: examining student exam scores, and using an evaluation instrument that tests a student's scientific reasoning ability.

Students in simulation rich discovery courses have routinely rated those courses as among their best courses. Scores for questions rating the overall course have been excellent, and in addition, when asked whether they preferred learning in the interactive environment used vs. a lecture-based course, 90% or more of students routinely said they preferred the methodology in the discovery based course. In the expository section of the surveys, they most often cited being able to learn for themselves or being able to explore a concept instead of just listening about it. Many students have noted that while they had encountered a concept in the an earlier (high school) course, they felt they gained a much deeper understanding of that concept through the discovery process.

We expect the largest impact of Chemland module use to be on a student's ability to derive concepts from data. We have begun a study of this using a scientific reasoning instrument developed at Hampshire College. The instrument presents the student with data (not related to chemistry) and asks questions that require students to formulate hypotheses, evaluate data for testing a hypothesis, interpret mathematical and statistical data, and interpret graphical information. This instrument became available to us during the Spring 1999 semester and we tested students at the end of their discovery-based general chemistry course. The control groups were: two classes at Hampshire College (one of Natural Science Majors students and the other of Non-Natural Science Majors) and a class from Mount Holyoke College that took a course in unified, cross-disciplinary science. Histograms showing overall scores for the scientific reasoning survey for each class are given in Figure 4.

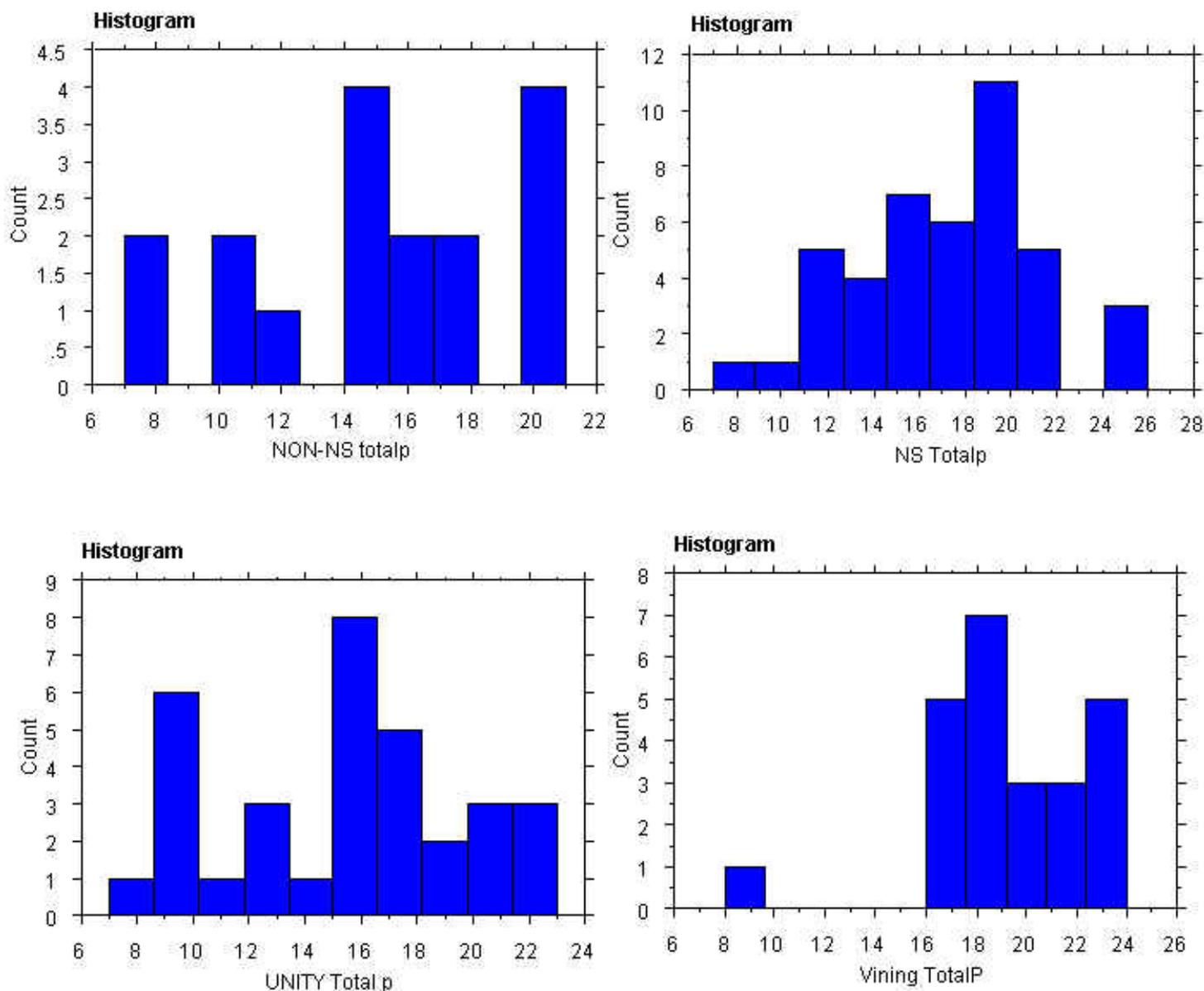


Figure 4. Histograms of overall scores on the Scientific Reasoning Exam. Top left and right are Hampshire College classes of Natural Science and Non-Natural Science students, respectively. Lower left is a Mount Holyoke College class in unified science and lower the lower right

Students in the UMass discovery-based class using Chemland modules performed significantly better than those of any of the control groups. Most noticeable is that all classes other than the UMass discovery-based chemistry course showed a wide range of scores whereas all students except one in the UMass class did very well on the exam. A more detailed analysis shows the students in the UMass class did particularly well on the portions of the exam that relate to assimilating data, testing hypothesis, and interpreting graphical data. Mean scores for each section of the exam are given in Table 2.

	UMass/ Chemland	Hampshire Natural Science	Hampshire Non- Natural Science	Mt. Holyoke Unified Science
Generating Hypotheses	4.58	5.04	4.24	4.58
Understanding and using Data	8.17	6.19	6.00	5.85
Mathematical and Statistical Reasoning	3.25	3.19	2.24	2.42
Interpreting	3.38	2.79	2.47	2.61

**Graphical Data**

Overall	19.38	17.21	14.94	15.46
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The UMass students did not perform significantly better on sections of the exam that tested formulating hypotheses or general mathematical and statistical reasoning. This is interesting in that the class is run in a way that presents the students with data and asks for interpretation. Much of the data is graphical and little is of a statistical nature. These data are consistent with our hope that the use of Chemland simulations in a guided inquiry environment lead to an increase in students' ability to analyze sets of data and come to useful conclusions.

During the Fall 1999 semester we conducted a similar study that showed students scores on the Scientific Thinking instrument increases after going through the discovery-based course. Over the same period, a similar group of students who had a traditional general chemistry course showed no statistical improvement.

**Conclusion and Availability**

We have reported here our experience with the software modules described. The enthusiastic response of both students and instructors has encouraged further development of Chemland. In the future, the authors will improve upon the modules currently available, making use of comments of users. We plan on continuing our study of the effect Chemland has on students' exploration and scientific thinking skills. In particular, spurred by our encouraging results, we are presently doing a comparative study observing the differences between using Chemland in class and as stand-alone homework assignments.

The Chemland installation program is available as an attachment to this article, and can also be downloaded from the author's home page, <http://soulcatcher.chem.umass.edu>. In addition, we have been converting the modules into Java applets for use on the internet. At present, 35 modules have been converted and may be accessed at <http://owl.chem.umass.edu/chemland/chemland.html>.

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**References**

1. R. W. Ricci, M. A. Ditzler, *J. Chem. Educ.*, 68, 228, 1991
2. M. A. Ditzler, R. W. Ricci, *J. Chem. Educ.*, 71, 685, 1994
3. A. M. Sarquis, *J. Chem. Educ.* 71, 506, 1994
4. S. R. Shadwick, R. S. Mohan, *J. Chem. Educ.*, 76, 1121, 1999.
5. S. R. McElveen, K. Gavardinas, J. A. Stamberger, R. S. Mohan, *J. Chem. Educ.*, 76, 535, 1999
6. S. A. Stewart, A. J. Sommer, *J. Chem. Educ.*, 76, 399, 1999
7. G. A. Rechtsteiner and J. A. Ganske, *The Chemical Educator*, 3(4), 1998
8. G. Bodner and W. Hunter, R. S. Lamba, *The Chemical Educator*, 3(3), 1998
9. C. J. Marzocco, *J. Chem. Educ.*, 75, 1628, 1998
10. D. Russell, C. Olson, S. Shadle, and M. Schimpf, *The Chemical Educator*, 2(1), 1997

11. R. W. Ricci, J. M. Van Doren, *J.Chem.Ed.*, 74, 1372, 1997
  12. R. M. Jarret, J. New, C. Patraitis, *J. Chem. Educ.*, 72, 457, 1995
  13. R. W. Ricci, M. A. Dizler, R. Jarret, P. McMaster, R. Herrick, *J. Chem. Educ.*, 71, 404, 1994.
  14. D. S. Burns, L. H. Berka, N. Kildahl, *J. Chem. Educ.*, 70, A100, 1993
  15. A. L. Parrill, J. Gervay, *J. Chem. Educ.*, 74, 329, 1997
  16. L. G. De Pelichy, E. T. Smith, *The Chemical Educator*, 2(2), 1997
  17. R. W. Ricci, J. M. Van Doren, *J. Chem. Educ.*, 74, 1372, 1997
  18. S. Toby, *The Chemical Educator*, 4(1), 1996
  19. S. Hinze, C. A. Wright, J. W. McGill, J. K. Gong, *The Chemical Educator*, 4(1), 1996
  20. B. L. Masson, *J. Chem. Educ.*, 73, 918, 1996
  21. M. Blackburn, *J. Chem. Educ.*, 72, 533, 1995
  22. D. E. Turner, *J. Chem. Educ.*, 71, 784, 1994
  23. M. Clark, J. S. Thrasher, *J. Chem. Educ.*, 67, 235, 1990
  24. T. de Jong, R. W. van Joolingen, *Review of Educational Research*, 68(2), 1998
  25. T. de Jong, R. W. van Joolingen, *Instructional Science*, 20, 389, 1991
  26. T. de Jong, R. W. van Joolingen, *Education and Computing*, 6, 241, 1991
  27. R. Kozma, J. Russel, *Journal of Research in Science Teaching*, 34(9), 949, 1997
  28. V. M. Williamson, M. R. Abraham, *Journal of Research in Science Teaching*, 32(5), 521, 1995
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