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Discovery Learning Using Chemland Simulation Software

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Abstract. We describe in this paper a set of computer-based simulations for use in general chemistry courses. We detail a discovery-based method of teaching, whereby students are led to discover concepts through guided-inquiry use of the simulation modules. Three methods of using the software are described, as is the development process we have employed. Finally, we describe our evaluation studies of the effects of our methodology and the use of a scientific reasoning instrument. The software is available free for download as part of this article.

Introduction

This paper describes a set of simulation programs for general chemistry and offers commentary on their use for enhancing the learning experience of introductory chemistry students. In traditionally taught general chemistry classes, students are taught the basic concepts of chemistry. This instruction is normally provided in the lecture portion of the course and may involve various degrees of active-learning strategies. Students are also taught how experiments are used to obtain scientific data by performing experiments in the laboratory section of the course [1–3]. In recent years laboratory experiences have often become more investigative, allowing students to design experiments to answer specific questions [4–14].

At the University of Massachusetts, we believe that these two parts of a course (lecture and laboratory) 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 believe the science's accepted concepts. Students rarely get the opportunity to analyze data and infer broader principles from trends that they may see in those data. In short, they do not fully have the opportunity to act as scientists. This limitation on the students' experience is not surprising because 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. There is rarely the ability of students to ask "What if?" and to test their question. A growing number of educators now make use of computer-based simulations to supplement student exploration in either their lecture or laboratory work [15–23]. The Chemland modules described here serve to bridge the gap between what is possible in the laboratory and what concepts are taught in the lecture; therefore, 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. We also hope to foster the ability of students to explore and discover beyond the specific scope of the general chemistry course, and are testing students to analyze this effect.

A number of educators have made use of simulation software in introductory courses. Some have attempted to aid students with different learning styles [1]. Others have made use of other types of discovery exercises both in and out of the classroom [2] and especially in the laboratory portion of courses [3].

The Chemland Software Set

Chemland, a suite of freely available 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.

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.

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.

Operation of the modules has been verified on a large variety of hardware platforms running Windows 95; Windows 98; and Windows NT, versions 3.5 and 4.0. Any user comfortable with a mouse and the Windows operating system should have no trouble navigating through and using Chemland. Brief instructions are provided for each module from a pull-down menu, which also provides the user with

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Table 1. Chemland Categories and Modules

Tools and reference	Thermodynamics	Properties of matter
Plotter	Specific heat	Gas laws
Periodic table	Calorimetry	Henry’s law
Units of concentration	Bond energy/heats of reaction	Gas phase boltzmann distribution
Molecular weight & weight percent	Gibb’s law of thermodynamics	Liquid phase boltzmann distribution
	Hess’s law	Equilibrium vapor pressure
	Heat transfer	Phases of the elements
		Enthalpy of dissolution
		Colligative properties
		Different gas laws
		Density of gases
Atomic structure	Basic tasks	Molecular structure and bonding
Mass spectroscopy	Solution making	Coulomb’s law
Atomic absorption and emission	Balancing equations	Molecular polarity
Electromagnetic spectrum	Significant figures	Bond length/energy
The photoelectric effect	Ionic compounds	Transition metal bonding
Orbital shapes	Oxidation numbers	Uv-vis spectroscopy
Quantum numbers	Molarity calculations	Metallic bonding
Orbital energies	Dimensional analysis	
Electron configurations	Elemental analysis	
Equilibria	Reactivity	Organic
Chemical equilibrium	Limiting reagents	Ph of organic molecules
Acids and bases	Rate measurement	Boiling point
Buffer ph	Rates of reaction	Heats of hydrogenation
Ph titration	Radioactive decay	Confirmational analysis
Ph buffer solutions	Electrochemical cell	Markovnikov’s rule
Le chatelier’s principle	Net ionic equations	Hückels’ rule
	Electrolysis	
	Ph of salts	

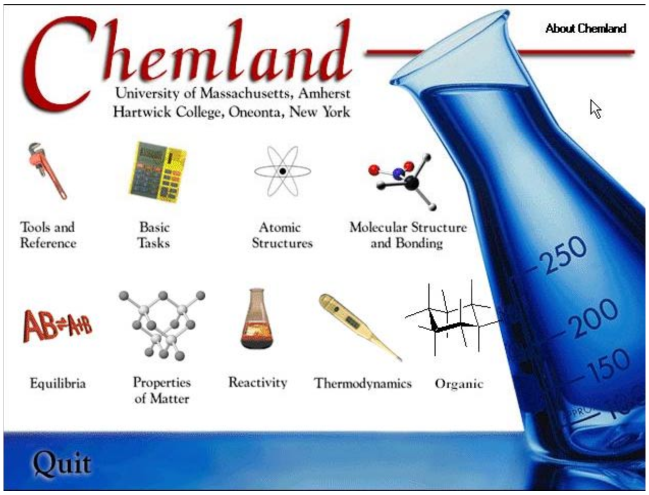

Figure 1. The Chemland main menu. Selection of each topic brings the user to a lower-level menu screen containing links to modules for that topic.

access to an interactive periodic table and a molar mass calculator.

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

For input, the user selects an element from the periodic table shown in the lower part of the screen. The feedback returned is not in the form of laboratory measurements, but rather as the experimentally determined ground-state electronic configuration as reported by Herzberg [25]. Atomic electronic configurations are presented 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. Or, one could allow students to explore this module for some length of time and discover the manifestations of 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, for example, how electron-electron repulsions affect the order of orbital filling. This redistribution of time results in more class time being spent on understanding the chemical and physical interactions responsible for the observed phenomena.

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

This module simulates a series of vapor pressure measurements. The measurement of vapor pressure is an experiment that could be performed in the laboratory 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 for study from a list of five and variation of the temperature. Feedback is provided as a measure of the vapor pressure of each liquid at the selected temperature. Students can use the simulation to explore boiling point, the relationship between temperature and vapor pressure, and effects of molecular

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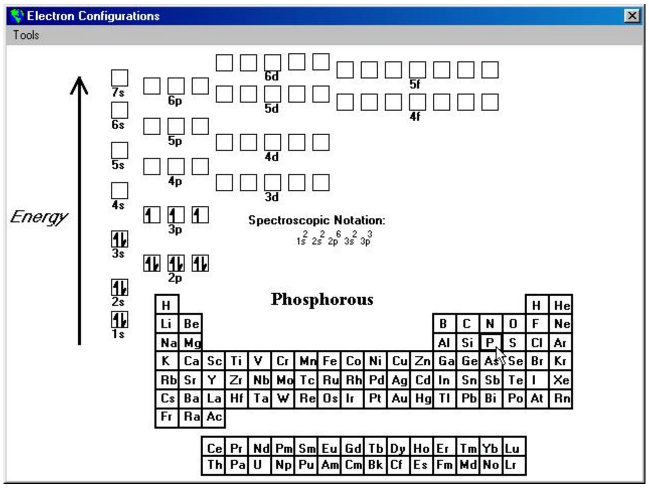
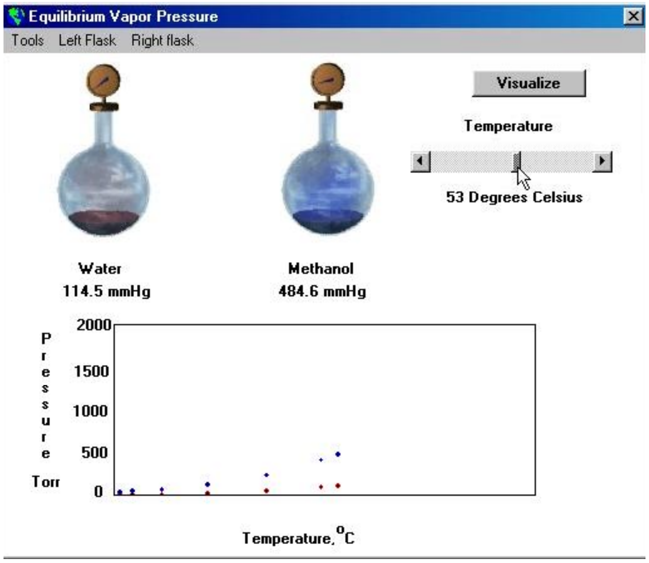


Spectroscopic Notation: $1s^2 2s^2 2p^6 3s^2 3p^3$

Figure 2. The simulation screen for the Electron Configurations Simulation Module. The element symbol for phosphorus has been selected.



Temperature: 53 Degrees Celsius

Water 114.5 mmHg

Methanol 484.6 mmHg

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

structure on these properties. The data obtained can also be used to calculate the enthalpy of vaporization for each liquid. In order to incorporate 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.

Throughout the Chemland suite, each module is written to encompass a single conceptual area through a simple interface. In addition to the interactive simulation, some modules are complemented by frames from animations showing a molecular scale interpretation of the concept. For example, the module on balancing chemical equations provides an animation after the reaction has been balanced by the student. The animation with voiceover shows and describes the breakdown of the written chemical formulas for the reactants into the correct number of each atomic symbol. The atomic symbols then rearrange to form the correct number of each product molecule, helping students to visualize the principle of mass balance, but not the actual mechanism of the reaction.

The Development Process

Chemland has been in use as an integral part of the general chemistry programs at the schools where it was developed—Hartwick College in Oneonta, NY and the University of Massachusetts at Amherst—for three years. In addition, approximately 600 colleges and high schools in the United States and overseas have obtained copies of the Chemland program. This 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 that 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.

One useful method of developing instructional software for use by undergraduate students is to involve those students in the development process. In this vein, undergraduate chemistry students have been included in every aspect of the development of the Chemland modules. The development of each module takes place in four steps:

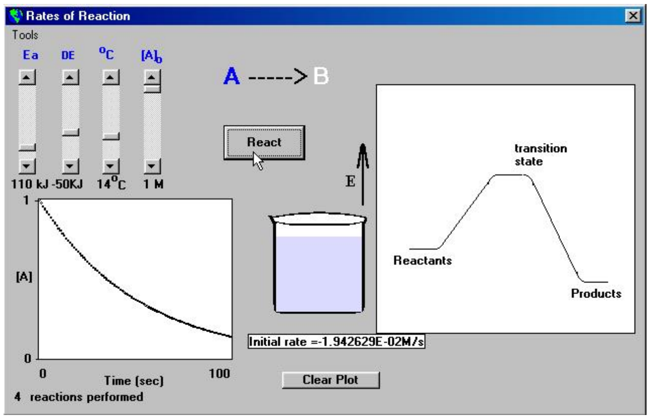
(a) Storyboard: A topic is selected for a module. We start with the question, “what would a student need to see to allow us to lead them to discover this concept?” We then design a module that will allow the student to explore and gain access to that information. The storyboard includes information about variables the student will manipulate, limits allowed by the program, underlying calculations, and the user interface.

(b) Programming: The module is developed as an independent, stand-alone program and is tested internally within our research group. The large majority of Chemland modules have been programmed by undergraduate chemistry students.

(c) Incorporation: Once the programs have been made and approved, they are incorporated into the overall Chemland program set. We have aimed to update the set about once each year, and currently distribute Version 6.0.

(d) Class testing: The programs are used in class and the instructor gains feedback from students as to their clarity and usefulness. This information is then used to make any necessary changes to the functionality of the modules or, in some cases, to simply eliminate a module from the program set.

We have chosen Visual Basic as our programming language for Chemland. Visual Basic offers an easy to use interface for designing user interfaces and coding screen objects. The same results can be obtained using C++, but we have found Visual Basic to be much easier for students to master. Students are trained to work on modules by starting with very simple programs that do more to teach them how to program than to develop a useful educational tool. We find, however, that 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 considering how we want to teach



110 kJ -50KJ 14^{o}C 1 M

Initial rate =-1.942629E-02M/s

4 reactions performed

Figure 4. Screen for reaction rates simulation.

something than we spend getting 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. The interactive software described provides a way for students to learn to think like chemists, that is 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 laboratory class in order to derive the chemical principles underlying those observations.

The individual modules within Chemland provide interactive simulations of various observable and unobservable phenomena at both the macroscopic and molecular levels. This allows the user to change experimental parameters and observe results. Furthermore, the software allows the students to perform experiments not feasible in the classroom and to then gather data and conclusions about these phenomena. For instance, the Radioactivity Module simulates and graphs the radioactive decay of four isotopes over very long time periods in order to help students derive and visualize the concepts of half-life and exponential decay. As such, 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. Our intent is that explanation and synthesis of the information obtained using the simulations is integrated into the method by which the instructor runs their course. The ability to use this method is intimately tied to effectively guiding the student through the simulations.

In 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 usually 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, showing students how to design and interpret broad studies. That is, we hope that students will both learn the content of chemistry and develop a higher level of critical thinking in general. We have preliminary 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. It is our hope that the following in-depth description of the contents and format, accompanied by examples of how we find Chemland to be most useful in teaching general chemistry, will encourage others to use it.

In-Class Use: Students with Computers. The Chemland software was originally designed to encourage learning through the in-depth 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 classroom equipped with computers for use by pairs of students.

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:

(a) a short (5 min) introduction to a topic by the instructor that defines what we will be studying, how it relates to other aspects of the course, and why it matters,
(b) an extensive exploration using the simulation where students are led to discover the relationships of interest. This portion of the class can take from 5 to 30 min, depending on the complexity of the material,
(c) a summation of the topic by the instructor.

About half the available class time is spent during the extensive investigation. This process 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 provide 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 comes from the students in the class.

At the end of this exploration, the instructor takes time to summarize the material. The summary serves to allow introduction of correct chemical terminology and to offer a “clean” set of notes for the students. This activity was instituted because our first attempts at teaching in this manner led to rather poor note taking by the students. For example, the module on rates of reaction allows the student to study a generic reaction by adjusting the energy of activation, the energy change for the reaction, the temperature at which the reaction occurs, and the initial concentration of the reactant. A screen capture of this module is shown in Figure 4.

The program plots a graph of time versus concentration of reactant based on the student’s input. An initial rate is calculated and a reaction coordinate diagram showing the energy of reactants, products, and transition state is displayed for each reaction as well. The student can change one or several of the above variables and a new kinetic trace will appear on the time versus concentration graph, allowing the student to compare the effects of a change of one of those variables on the rate of reaction. In analyzing and comparing these plots and recorded initial rates, the student can uncover the relationships between the above variables and the rate of a reaction. The student can also discover that the reaction modeled is first-order and can potentially discern the Arrhenius equation.

We have found this simulation too complex for students to study without substantial guidance, because of the large number of variables available to alter. The students are, therefore, led to first explore the effects of initial concentration. They quickly find that the initial rate is proportional to that concentration. They are then asked to explore the effects of temperature and find that as temperature increases, so does reaction rate. They then study activation energy and are finally asked to predict what effect the overall change in energy will have and then use the simulation to corroborate or refute their predictions. Data from the simulation can be used throughout the remainder of the kinetics topic, but we also find it useful to use data obtained by students in the laboratory to support the exploration process.

Occasionally students will be knowledgeable about a topic prior to encountering it in class. This has the danger of allowing them to head off the exploration process for the other students. We avoid this by carefully wording our requests, using phasing such as “I want you to discuss these results and then tell me why they occur,” as opposed to simply asking for student impressions as to why they occur. Although some students want to answer right away if they know the material, they quickly become aware of how the class works.

In-Class Use: Instructor Presentation. Although less ideal, we have used the Chemland simulations in large-lecture formats, where the instructor has use of a computer that is projected. In these cases, the students cannot perform their own explorations. We have found in these cases that the most effective use is a mixture of demonstration and as a tool to test predictions. In this case, the instructor uses the simulation to show a set of data. The students talk in small groups to develop conclusions based on the data. The instructor then asks the students to predict what will occur if the simulation is probed in other ways and then tests those predictions.

This is a good method for giving the students partial control of their own learning and for developing an understanding from data, but it does not give them experience in performing explorations. In order to foster that part of the experience, students can download the programs and use them at their leisure outside of class. This is described further in the next section.

Outside of Class: Exploration Assignments. Because we teach very large numbers of students each year, we are particularly interested in determining if tools of this type can be effective in settings where no direct instructor–student interaction takes place. In leading students through the chemical principles underlying these modules, the Chemland software attempts to teach students the process of how scientists, or more specifically chemists, think. It should be possible to offer the guidance for a rich and controlled exploration experience by presenting students with questions outside of class. In order to mimic what an instructor would do in class, instant feedback must be offered in analysis of the student’s answers. The discovery process will be hampered if the student progressed through a series of questions without understanding the answer to each one along the way. We are currently studying the effectiveness of using an electronic homework system (the On-Line Web-Based Learning, OWL, system developed at UMass) to sequentially deliver these questions and to offer appropriate feedback. The system grades and answers each question as it is answered and gives a detailed explanation of the correct answer. Samples of these assignments with appropriate feedback are offered in the supporting materials (510031wvs1.pdf) to this article. We will detail on this portion of the project in a future report.

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 [26–30]. It is our belief that the use of Chemland discovery modules helps ground students in a firm understanding of concepts, and this should positively affect their problem-solving skills. The modules, however, 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 examination scores and using an evaluation instrument that tests a student’s scientific reasoning ability [31].

Over a period of six years (three at Hartwick College and three at UMass), we have run courses using the discovery modules side-by-side with standard lecture-based courses. In the discovery courses students used computers at their desks and the class sessions were run in a guided-inquiry fashion. In each of these years, students in the discovery sections performed better overall than those in the traditional lecture sections, usually by a margin of 0.7 to 1.0 GPA units out of 4.0. This analysis, however, may be misleading or at least not conclusively attributed as effects of course methodology. In each comparative instance there exist a number of factors that could affect student performance. The most obvious is class size. By technical limitation, courses that use discovery methodology are relatively small, from 20–50 students. Traditional lecture sections are normally much larger, from 100–170 students. A further complicating factor is student course selection. Students enrolled in the small, discovery sections are often more interested in becoming chemistry or biochemistry majors than those in the larger, traditional sections. In addition, students in the smaller classes often have somewhat better chemistry preparation than those in the large lecture sections. Therefore, although we are pleased and encouraged by student performance in the discovery courses, we cannot conclude that the higher scores of students in those sections are attributable to the use of the Chemland simulations and a discovery methodology. We are encouraged that this year, due to scheduling of honors students, there are a number of similar students in both the discovery courses and

Table 2. Mean Scores for Each Section of the Exam

	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 graphical data.	3.38	2.79	2.47	2.61
Overall	19.38	17.21	14.94	15.46

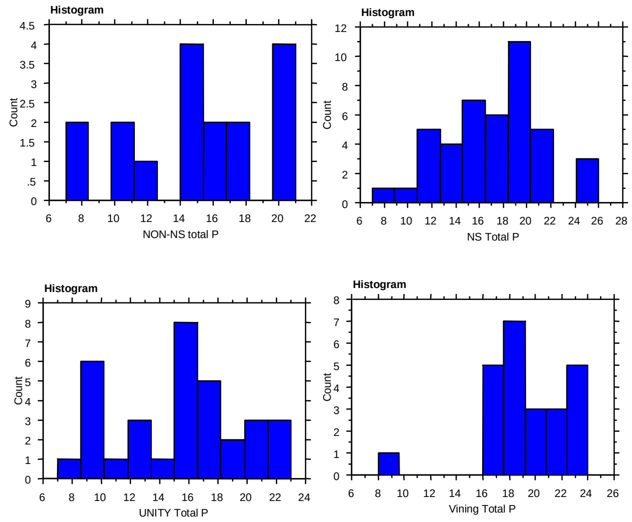


Figure 5. Histograms of overall scores on the scientific reasoning survey. Top left and right are Hampshire College classes of natural science (NS) and non-natural science (NON-NS means that students were not enrolled in any science that semester) students, respectively. Lower left is a Mount Holyoke College class in Unity of Science and the lower right students in the UMass discovery-based class using Chemland modules.

the larger lecture courses that will make comparisons more meaningful and fruitful.

When we look just at the students in the simulation-rich discovery courses, we find that they have routinely rated those courses as among their best academic experiences. Scores for questions rating the overall course have been excellent, and, in addition, when asked whether they preferred learning in the interactive environment used versus 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." For this reason we believed that it was wise to find out if the students actually performed better in these courses as well as liking them better.

We expect the largest impact of Chemland module use to be on a student's ability to derive concepts from data. We have, therefore, begun a study of this effect using a "scientific reasoning" instrument developed at Hampshire College. The instrument presents the student with data (not directly related to chemistry, but rather generic in scientific information) 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. We compared these results to the post-scores only on control groups tested in the prior semester. This included two classes at Hampshire College (one of natural science majors students and the other of non-natural science majors) and an inquiry-based class from Mount Holyoke College in unified, cross-disciplinary science. All students were in their first year of study at a college. Histograms showing overall post-course scores for the scientific reasoning survey for each class are given in Figure 5.

Students in the UMass discovery-based class using Chemland modules showed a higher level of performance overall on the post-test than those of any of the control groups. A noticeable difference is that all classes other than the UMass discovery-based chemistry course showed a wider range of final scores whereas all students except one in the UMass class scored at the 16 or above level out of a possible 29. (It should be noted that the Natural Science class at Hampshire showed significant pre–post change on the survey). 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.

The UMass students did not perform significantly better on sections of the exam that tested formulating hypotheses or general mathematical and statistical reasoning. This result 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 leads to an increase in students' ability to analyze sets of data and come to useful conclusions.

Future Work

Although our evaluations to date are encouraging, we can not as yet prove a direct benefit of our teaching tools or methodology. The initial data presented only looked at test results after the course and can, therefore, not take into consideration the level of ability and understanding of students at the beginning of the class (i.e., we do not have a pre–post comparison for the group or initial baseline). For this reason, we are currently performing pre- and post-course testing and analyses of large sets of students using Chemland modules in a guided-inquiry environment as described here, and we will examine our results for changes in students' abilities. This will include an analysis of similar sets of students within the UMass Chemistry department based on major, SAT scores, and test scores, and also compare them to similar groups at Hampshire College and Mt. Holyoke College. We are also performing a comparison between the use of the modules in class versus their use by students over the Internet where they are led through module use by an electronic homework system that asks questions and gives general feedback before they continue the investigation.

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 the comments of users. We plan to continue 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 supporting material to this article (510031wvs2.zip); it can also be downloaded from the author's home page [24]. Because the installation files are rather large (approximately 25 Mb) the authors will, upon request, send a CD-ROM, free of charge, that contains the installation software. 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 on the World Wide Web [32].

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