The *Virtual ChemLab* Project: A Realistic and Sophisticated Simulation of Inorganic Qualitative Analysis

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Chemistry is a laboratory science and as such it requires that students participate in meaningful laboratory experiences. The fundamental purpose of these instructional laboratories is to (i) provide “practical experience” by connecting the “theory” taught in the classroom with the “real world” of the laboratory, (ii) teach laboratory technique, and (iii) teach the cognitive processes (or analytical skills) that form the foundation of chemistry and other laboratory sciences (1). In actuality, however, a significant fraction of students go through these laboratories with little thought about what they should learn, but narrowly follow the written directions for an experiment to get the expected results (affectionately called “cookbooking”). The reasons for this are many, but certainly a prime factor behind this tendency to “cookbook” is the rigidity imposed upon instructional laboratories by severe time constraints, large numbers of students, costs, environmental considerations, and safety considerations (2, 3).

An attractive solution to address many of these issues is to develop realistic computer simulations of laboratory experience. It is beyond the scope of this article to provide a critical review of the simulations that have been either produced privately or commercially, but it is sufficient to say that the effect of these simulations has been minimal because (i) the software interface is either too simplistic or too cumbersome (4, 5), (ii) the range of problems or outcomes for the student is restricted or small in scale (4, 6), or (iii) there is not an adequate method to give assignments or to assess performance on those assignments (6).

While these software packages may offer significant contributions, we believe that the next breakthrough in chemistry instruction lies in the development and use of realistic computer simulations of complex chemistry experiments (both quantitative and qualitative) that reinforce concepts taught in the classroom, do not limit student interaction or student thought, provide an environment for creative learning, have a consistent, intuitive interface, and allow instructors to give assignments and appraise student performance easily (2). We foresee three important advantages of having access to these types of simulations: (i) increased learning opportunities, (ii) improved access to instructional laboratories, and (iii) reduced costs and environmental effects.

In the past five years, we have created a set of sophisticated and realistic laboratory simulations for use in freshman- and sophomore-level chemistry classes and laboratories called Virtual ChemLab. We have completed simulations for Inorganic Qualitative Analysis, Organic Synthesis and Organic Qualitative Analysis, Experiments in Quantum Chemistry, Gas Properties, Titration Experiments, and Calorimetric and Thermochemical Experiments. In this article we will describe our first simulation, Inorganic Qualitative Analysis, demonstrate how we used it, provide a detailed assessment of student responses, and describe its pedagogical utility.

The Simulation

**General Principles**

Before describing the inorganic simulation in detail, it is important to understand the general scope and intent of our simulations. As mentioned earlier, the purpose of instructional laboratories can be summarized as (i) connecting the theory of the classroom with the practice of the laboratory, (ii) teaching laboratory technique, and (iii) teaching cognitive (or analytical) thinking skills (1, 2). Of these purposes, we believe it is very difficult to create a simulation with sufficient detail and realism that it can effectively teach laboratory technique. We believe that laboratory technique must be experienced first hand in the laboratory with real equipment. Laboratory processes or sequences can be simulated, but laboratory techniques should be taught in an actual laboratory setting where students can handle the actual laboratory equipment and chemicals.

For this reason, in the Virtual ChemLab set of simulations, our purpose is not to teach laboratory technique. Our simulations gloss over the “how” of performing specific laboratory functions and, instead, focus on the “what”, “when”, and “why” of experiments. That is, our instructional focus lies on the other two purposes stated earlier: to connect theory with practice and to teach cognitive thinking skills. To do this adequately in a simulation, students must be presented with a completely open-ended environment where they are free to make the decisions and experience the resulting consequences that they would confront in an actual laboratory setting.

Our goals, therefore, in each Virtual ChemLab simulation are to: (i) provide a realistic laboratory environment on the computer where students can psychologically feel they are in a laboratory setting; (ii) provide an easy-to-use interface that is intuitive and quickly learned; (iii) provide an open-ended, unrestricted simulation that allows students to make the decisions they would make in an actual laboratory setting; (iv) provide realistic outcomes using real pictures or videos when possible; and (v) provide instructors a method to make assignments and evaluate student results.
Simulation Description

Virtual ChemLab is written in Director, a programming language produced by Macromedia that can be run on both PC Windows (Windows 95/98, NT, 2000, ME, etc.) and Macintosh OSX platforms. Virtual ChemLab is self-contained and requires no other software except for a QuickTime plug-in which is common to almost all computers. Although Director, in general, can be configured to run through a Web browser using Shockwave, Virtual ChemLab is too large to deliver over the Web and, instead, runs as a standalone executable.

The Virtual ChemLab general chemistry set of simulations are licensed to Prentice Hall and are divided into two products: a full site-license version and a student version. The site-license version is intended to be a server-based installation, although it can be installed as a standalone product on individual computers. The server-based installation stores a centralized database that contains student lists, passwords, assignments, student lab books, and scores on the server; it is meant to be installed on various client computers connected to a server. This version allows instructors to import classes, make assignments, view student lab books, and export scores. At the same time, the server version allows students with access privileges to login to the laboratory, explore different laboratories, and perform assignments. Students can also record notes and observations and report their answers in a lab book.

The student version of the software contains the full laboratory simulation and can be installed on one computer. The only difference between the client version and the student version is that the student version does not access a centralized database. This means that an instructor cannot electronically give the student assignments, and the user cannot electronically report findings to the instructor. The student version is intended to be more of an exploratory and discovery tool; however, workbooks are provided so that an instructor can give paper assignments.

A detailed description of the inorganic simulation itself is beyond the scope of this article, but more information can be found at http://chemlab.byu.edu (accessed Jul 2004). However, the general features of the simulation include 26 cations that can be added to test tubes in any combination; 11 reagents that can be added to the test tubes in any sequence and any number of times; necessary laboratory manipulations including centrifugation, flame tests, decanting, heating, pH measurements, and stirring; a lab book for recording results and observations; and a stockroom window for creating test tubes with known mixtures, generating practice unknowns, or retrieving instructor-assigned unknowns. The simulation uses over 2500 actual pictures to show the results of reactions and over 220 videos to show the different flame tests. With 26 cations that can be combined in any order or combination and 11 reagents that can be added in any order, there are in excess of $10^{16}$ possible outcomes in the simulation.

To achieve our goal of having an open-ended simulation with real outcomes yet keep the simulation at a manageable size and complexity, a few assumptions and restrictions have been applied: (i) The cations are the nitrates and are dissolved in water to form a $0.02 \text{ M}$ solution except for $\text{NH}_4^+$, which is a $1 \text{ M}$ solution. (ii) Additional cations cannot be added once the test tube is in the laboratory. (iii) The reagents have concentrations of $3 \text{ M}$ for $\text{HNO}_3$, $\text{NaOH}$, and $\text{NH}_3$, $0.1 \text{ M}$ for the $\text{Na}_2\text{S}$, $3\%$ for the $\text{H}_2\text{O}_2$, and $1 \text{ M}$ for the $\text{NaCl}, \text{Na}_2\text{SO}_4$, and $\text{Na}_2\text{CO}_3$ solutions. (iv) The $\text{pH}$ 4, pH 7, and pH 10 solutions are inert buffers and are added in sufficient quantity to set the pH of the solution to the indicated value. (v) Reagents are added in excess. (vi) After decanting, precipitates are rinsed with an appropriate solution so the precipitate does not dissolve. Except for these constraints, students are unrestrained in the order and combination of the reagents they add to any cation combination. The database and algorithms used to determine the chemical outcomes and pictures used in the simulation are based on actual chemistry that has been performed in the laboratory and have been extensively tested.

Evaluation and Assessment

Introduction

A team of evaluators conducted an extensive assessment of the Inorganic Qualitative Analysis simulation using online surveys sent to over 1400 students enrolled in freshman-level chemistry courses between January 2001 and April 2002. These online surveys consisted of Likert-type questions, free response questions, and descriptive information (such as: gender, computer literacy, year in school, etc.). Additionally, we conducted “think-aloud” interviews with 26 students who used the program, and on several occasions we observed students in the computer lab while they were working on virtual assignments. We analyzed data from the online surveys through descriptive statistics and by conducting several analyses of variance (ANOVAs) and linear regressions. To properly measure the results of the simulation-based learning, we coded data from interviews and observations and categorized them for generalization purposes, so that our results would measure “implicit application” of the learned material (7).

While much of our evaluation and assessment focused on student opinion as expressed in our surveys and direct observations, we found that some of our most interesting observations and findings occurred when we correlated student opinion and performance with each student’s personality profile. The personality profile of each student was determined using the well-established personality test called the Herrmann Brain Dominance Instrument (HBDI) (8). The HBDI generates 12 numerical values to represent various preferences. We found that two of the numerical values returned by the HBDI, the cerebral and limbic scores, correlated remarkably well with many of our observations.

A brief summary of the tendencies shown by the people with high cerebral or limbic scores is instructive. Someone with cerebral preferences “can understand nonlinear thinking and verbalize it…. They can switch from fact-based, rational functioning to experiential modes” (8). Someone with limbic preferences “is characterized by very strong preferences in conservative thinking and controlled behavior with a desire for organization and structure as well as detail and accuracy” (8). People that have high cerebral scores typically choose professions of design engineers, research scientists and development scientists; people that have high limbic scores typically choose professions in nursing and other disciplines in the “helping profession” with a heavy administrative load.
We found, within a 99.9% confidence interval, that the higher percentage of students said that they liked the inorganic simulation because: (i) it allowed them the freedom to explore, (ii) it allowed them to focus on underlying chemistry principles, (iii) it allowed them to repeat procedures, and (iv) it was easy to use and navigate. We also discovered from instructor interviews that instructors like the inorganic simulation because they can flexibly integrate it with the existing instruction. In the section below, we describe in more detail each of these five major categories.

Results

Freedom To Explore

Students liked the inorganic simulation because they were free to explore in a safe environment. One student said, “I just liked that I could waste supplies and do things over again. It was also nice to mess around on my own.” The way students “mess around on their own” varies according to individual learning styles, as we discovered through multiple observations and interviews. Some prefer to systematically try all of the possibilities and write flow charts to document their effective cation isolation strategies. Others employ a hit-and-miss strategy and mentally take note of their isolation strategies. Some students demonstrate confidence in their knowledge of general chemistry principles, while others are much more cautious (as shown by making decisions slowly, or asking questions like “Is this what you would do here?”). Some students benefit from this new freedom to explore, but other students do not. Another question we asked 208 students in the evaluation of Virtual ChemLab was: “Please mark your agreement with the following statement by choosing a number from 1 (strongly disagree) to 7 (strongly agree). I would like more guidance in using ChemLab: Inorganic.”

We found, within a 99.9% confidence interval, that the higher someone’s cerebral score (creative learner), the less help they feel they need in using the inorganic simulation, and the higher someone’s limbic score (structured learner), the more help they want in using the inorganic simulation (Figure 1). Therefore, we can say from our evaluation that structured learners (such as premedical or predental students) would want and need more guidance performing assignments using Virtual ChemLab than engineering, chemistry, or physics students.

Although some students like exploring chemistry topics in a safe environment, we discovered that structured students (those with higher limbic scores) spend less time exploring on Virtual ChemLab. Within a 95% confidence interval on a sample size of 202 students, students with higher limbic scores report that they spend a smaller percentage of time exploring or conducting “what if” experiments in Virtual ChemLab (Figure 2). These students want to have someone (or something) close by to guide them in experimenting in Virtual ChemLab, and they also are much less likely to try new procedures on their own. This study shows that these types of students have a much harder time experimenting in Virtual ChemLab, and we also believe that these same students will have difficulty learning in any loosely structured learning environment, not because they are incapable, but because of their individual learning preferences. They need additional support and guidance to learn effectively in these more open-ended learning environments.

Focus on Underlying Chemistry Principles

Perhaps the largest educational benefit of the inorganic simulation is that students can focus on the principles of general chemistry, rather than focusing on troubleshooting aspects in a laboratory setting. These troubleshooting aspects imply more than just laboratory technique. Laboratory technique focuses on how to do something, whereas the troubleshooting aspects focus more on why something does not happen the way it should. One of the reasons beginning chemistry students feel overwhelmed in their first laboratory class is because, we believe, they are consumed by the details of lab technique and the troubleshooting aspects in the laboratory. For example, just because a student remembers how
to test the pH of an aqueous solution does not mean that he or she tested the pH of the *correct* solution. The inorganic simulation eases this educational burden for students by allowing the student to focus on the *what* of an experiment instead of the *how*. We believe that learning the *how* is vitally important, which is why we believe Virtual ChemLab is best used with a “wet” laboratory.

While the inorganic simulation cannot teach a student the important skills of using and manipulating equipment (the *how*), we found that it does help students apply chemical principles by allowing them to repeat procedures, explore, and reinforce their understanding of chemical theory in an open, unrestricted, and realistic environment. When asked on a survey how her problem-solving strategy had changed using Virtual ChemLab, one student said, “I found that trial and error is a viable option, and I was much more apt to run several trial runs since they were easier to do than in a wet lab.” Another student said that the inorganic simulation helped him focus on the underlying chemistry principles, saying, “I like the fact that it is much faster than if we were to physically do the lab. It is also is interesting to try a bunch of experiments while they are all fresh in your mind and have them work out quick so you can fully analyze everything all at once and recognize the main point.” For the first time, these students learned the value of trial and error and of gathering and analyzing multiple pieces of data in a chemistry experiment to decide which experimental procedures will achieve the desired result.

When students narrowly focus on the steps (or the *how*) of an experiment, they “cookbook” where creating the final product becomes more important than making connections with chemical theory. Drawing connections with principles of chemistry (the *what* or the *why* of an experiment) is the thinking aspect of a laboratory. This is something chemists do intuitively and is the basis for their expertise; however, students must be taught to “think like chemists” in order to develop expertise. To determine whether Virtual ChemLab helps students understand the *what* and *why* of an experiment, we asked: “On a scale of 1 (strongly disagree) to 7 (strongly agree), mark your agreement or disagreement to the following statement. ‘When I use ChemLab: Inorganic, I am more confident in my ability to think like a chemist.’” Our results are shown in Figure 3. Nearly 50% of the students reported agreement with this statement by marking a 5, 6, or 7 on the scale. Although the average of all student responses is 4.21, the students who were in school longer responded more negatively to this question than students who had not (99.9% confidence level). (The average with freshmen was 4.86, sophomores’ average was 4.53, juniors’ average was 3.67, and seniors’ average was 3.46.) Based on years of experience in this course, we believe that the upper-level students reacted more negatively to this question because they were reacting to the freshman-level course, not the program itself.

**Ability To Repeat Procedures**

Students liked the virtual reactions in the inorganic simulation because they were quick, consistent, and easily interpretable. Eighty-two students (out of 262) in the open-comment section of the survey said that they liked being able to run experimental procedures multiple times. Unlike the wet laboratory, students were more confident in the results they obtained because they were sure that the virtual test tube was not contaminated. Examples of these comments include, “I like the ability to get through the experiment quicker. If you mess up it is easier to start over. It allows you to see what will happen without all the dangerous interactions with the chemicals.” Another student said, “If you make a mistake, you don’t waste material—you can just start over again.”

To demonstrate how students can run experimental procedures multiple times, one student said during an interview that he went through 8 practice unknowns for one of his virtual assignments. When he was asked how many practice unknowns he went through on a previous virtual assignment, he said, “I like the ability to get through the experiment quicker. If you mess up it is easier to start over. It allows you to see what will happen without all the dangerous interactions with the chemicals.” Another student said, “If you make a mistake, you don’t waste material—you can just start over again.”

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he counted them up from his paper and identified 15 or 16. The student said he did so many practice unknowns so that he could be sure his flowchart (his stepwise guide to identify how the chemicals reacted) would work correctly. In fact, he had written two different flowcharts to identify his unknown for one of the assignments. Because this student was able to repeat his procedures, he could experiment with multiple practice unknowns. He became very confident in his two flowcharts. He had learned the correct set of steps (the how) to identify any one of the seven cations in his virtual assignment and was then able to focus on underlying chemistry principles and trends (the what and why). However, if he was in a wet laboratory, time, cost, and other resources would not have allowed this exploration to occur.

**Ease of Use and Navigation**

When students were asked what they liked about the virtual lab, more than anything else, students liked the appearance of Virtual ChemLab. This also parallels one of the questions on our survey: “Please mark your agreement with the following statement by choosing a number from 1 (strongly disagree) to 7 (strongly agree). ‘I like the appearance and layout of Virtual ChemLab.”’ Over 70% of the students agreed with this comment by marking a 5, 6, or 7 (Figure 4). The most common reason students gave for liking the inorganic simulation in the open-response section of the survey was because they thought the program was easy to use. Some students said that the layout and interface were intuitive; others thought that the program was fun. Still others said that the inorganic simulation was easy because it provided them the learning support they needed while they used the program. To further clarify this assertion, we included some common student responses about why they liked the inorganic simulation. One student said, “I like the appearance. It looks like a fun game.” Another said, “In general, I don’t like chemistry at all, but I actually had fun using ChemLab, and that really surprised me. It was nice not to have to wash out beakers and spill stuff all over the place.” Another student said, “I like the help guide that shows you what reactions are taking place in the test tube.”

We also found that students’ personality profiles influence how they perceive the program. Two more numbers generated by the HBDI indicate left-brained and right-brained preferences. Left-brained preferences would indicate people who are “verbal and structured in their thinking, efficient, time-oriented, linear, and precise” (8). People who have high right-brained preferences would be “intuitive, nonlinear, experientially oriented, and sensitive to beauty” (8). Using these two personality preferences, we conducted an analysis of variance with the responses to the “appearance of ChemLab” question, and, within a 95% confidence interval, we discovered that people who like the appearance of the inorganic simulation have stronger left-brained preferences. People who do not like the simulation’s appearance have stronger right-brained preferences (Figure 5). In more general terms, people in technical fields, science, engineering, and manufacturing would like the appearance of the simulation more than writers, artists, musicians, psychologists and counselors (8).

These same left- and right-brained preferences influence students’ levels of satisfaction with Virtual ChemLab. A generic question, such as, “Please mark your agreement with the following statement by choosing a number from 1 (strongly disagree) to 7 (strongly agree). ‘I am satisfied with ChemLab: Inorganic,” is a question that measures students’ overall impressions. From this question, we found, within a 95% confidence interval, that the greater someone’s left-brained preferences, the more satisfied they are with the inorganic simulation. In other words, students who are linear, structured in their thinking, and precise are more satisfied with the simulation. We also discovered that the greater someone’s right-brained preferences, the less they prefer the appearance of the inorganic simulation. These students who are intuitive, nonlinear, and experientially oriented are not as satisfied with Virtual ChemLab (Figure 6).

**Flexibility with the Instructional Implementation**

We also conducted a formal case study with 152 students enrolled in a freshman honors general chemistry class at Brigham Young University. From this case study, we learned how important implementation of Virtual ChemLab is in the classroom. During this case study, we gave all the 152 stu...
udents three different “unknowns” or assignments. In the first assignment, we gave them a description of the chemistry and a complete separation scheme to help them determine the cations in their unknowns. In the second assignment, using a different set of cations, we provided a description of the chemistry they would need to determine their unknowns, but did not provide them with a separation scheme. In the third assignment we did not provide either a separation scheme or a description of the chemistry.

We discovered that Virtual ChemLab was easily integrated into the existing course material. In fact, not only were our previous findings confirmed in this case study, but we were also able to identify which students were (and were not) comfortable in the learning environment of the program and with the implementation strategy described. Previously, we stated that the more cerebral students need less help in learning how to use the program. We were able to confirm that these types of students were more comfortable using the inorganic simulation and that these students were more comfortable with the instructor’s implementation strategy. In this study, we conducted an analysis of variance with cerebral scores and time spent completing the third experiment (the experiment with no guidance provided), we discovered within a 95% confidence interval that the honors students who had a higher cerebral score spent less time on an experiment that did not provide any instructional procedures (Figure 7).

Discussion

From our results above, we discovered four guiding principles that other researchers and educators can employ when using a computer simulated learning environment, such as Virtual ChemLab, in their classroom. (i) Students learn better when “hands on” laboratory instruction is coupled with simulated laboratory instruction because students have another representation of chemical phenomena. (ii) Beneficial software programs give instructors the flexibility to create experiments according to the needs of their students, and, for various reasons including saving time and creating less laboratory mess, students like this new flexibility. (iii) Different types of learner support are utilized by different types of students. In general, students in preprofessional programs (like predental or premedicine or nursing) need and want a high level of structure and learning support, while others (like engineering, chemistry, and physics students) do not. (iv) Student opinion about a software program is influenced by many different factors. For example, different types of students report different levels of satisfaction. This means that to truly value the worth of a software program, instructors should also consider learning preferences and personalities when interpreting the results of their findings. We will discuss each of these below.

Students Learn Better

From our surveys, observations, and interviews we have repeatedly found that the most effective use of Virtual ChemLab was as a lab supplement. For example, we found that students used the virtual laboratory environment to explore and experiment in a way that would not be possible or practical in a wet laboratory environment. Many students reported that ChemLab increased their understanding of the subject matter and improved their ability to “think like chemists”. We also observed similar findings when the software was used as a supplement in a classroom setting.

Flexibility in Implementation

Flexibility is another key dimension of effectively using educational simulations. Indeed, chemistry software programs that are highly flexible benefit both instructors and students. Instructors can create experiments according to the needs of their students and according to their instructional goals. Students can learn material in ways that fit their own learning styles: to explore and experiment freely, and reproduce their procedures multiple times for reinforcement purposes. When software programs are coupled with a good implementation strategy that considers personality styles, teaching students underlying chemistry principles is feasible and beneficial to students.

Different Types of Learners

Additionally, accounting for diverse learning styles is important to successful implementation of educational software. Among other things, this is significant because students

Figure 6. Levels of satisfaction with Virtual ChemLab as a function of HBDI left- and right-brain scores (1 = very unsatisfied; 7 = very satisfied).

Figure 7. Time completing assignment #3 (no instructional support provided) as a function of HBDI cerebral scores.
prefer different levels of structure and guidance based on their personality styles. Some students can run experimental procedures multiple times and can quickly learn from their findings, others can spend so much time running ineffective procedures that they can get frustrated. In education, there is a delicate balance between utilizing exploratory teaching techniques, and, at the same time, minimizing frustration. To effectively use any computer simulation, it is important to provide helpful resources to students if, and when, they reach the boundaries of their knowledge. If this is not done, there is a mismatch between the instructor's teaching style and the students' learning preferences, and because of this mismatch, neither will be as successful as possible. Examples of helpful resources include, but are not limited to: having teaching assistants available to answer questions, providing a list of “Frequently Asked Questions” to students, providing tutorials, and giving in-class instructions and demonstrations. It is also beneficial to have instructors and teaching assistants available during consultation hours. When using computer simulations in education, effective learner support needs to vary enough to facilitate different learning styles. We have implemented many of these strategies and have found a marked improvement in the satisfaction level of our students using Virtual ChemLab based on some preliminary studies.

Differences in Satisfaction

This last finding is significant because, when evaluating the educational worth of any instructional material for chemistry courses, the evaluation needs to include more information than “An average report of satisfaction for ‘Product X’ is 4.73 on a 5.00 scale.” Judging the significance of a software program is more complex than that. Many factors influence why students may report dissatisfaction with a piece of software: poor computer literacy, a lack of student–teacher interaction, personality styles, learning preferences, et cetera. When reporting the educational worth of a software program, instructors and researchers should try to identify and account for anomalies, and they should modify their instruction to help those less successful students improve.

Conclusion

When simulated chemistry laboratories are implemented effectively, students can have additional opportunities to engage in meaningful pedagogical experiences. Through our evaluation of the inorganic Virtual ChemLab we have found that if effectively used it (i) provides “practical experience” by connecting the “theory” taught in the classroom with the “real world” of the laboratory, (ii) provides a realistic learning environment for different learning styles, and (iii) teaches the cognitive processes (or analytical skills) that form the foundation of chemistry and other laboratory sciences (1). Additionally, we have found that this simulated learning environment helps overcome the tendency of students to “cookbook” by reducing many of the constraints of wet labs including costs, environmental considerations, and safety considerations.

Literature Cited