

Using Simulations to Transform the Nature of Chemistry Homework

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Introduction

Because introductory chemistry is abstract and often seems distant from students' experiences, instructors find it difficult to bridge the gap between theory and real chemical processes in a way that promotes interest in the subject, and thus an intuitive understanding and long-term retention of the material. Our starting point is that paper-and-pencil homework is simply not well suited to this goal and, while hands-on laboratory activities are important, they are typically limited in number and flexibility due to time, cost and safety constraints. Furthermore, introductory chemistry courses are typically large courses that are often viewed as essential to the department and university's mission, and therefore not to be experimented with lightly. In this paper, we outline our strategy for designing simulations and integrating them smoothly into currently existing introductory courses, in order to gradually improve student learning.

Current computer-based instructional support in chemistry addresses some of the teaching/learning difficulties by relating concepts to meaningful and motivating contexts, by making them more concrete and visual, and by promoting active learning. For instance, by coupling acid-base chemistry to *n*-type and *p*-type doping of semiconductors, students can be given a broader view of the nature of thermal equilibrium.¹ A number of curricula are evolving to make stronger connections to real-world contexts via case studies from environmental studies and materials science.^{2,3} Our group has also created software that contextualizes introductory chemical concepts, including our "Acclimatizing on Everest" and "Internal Combustion Engine" applets⁴, in order to supplement homework on topics such as equilibrium and thermodynamics. In addition, a wide variety of tools are available to improve visualization at the atomic and molecular levels, and to expand active learning. Software is also available for simulated laboratories on specific topics like kinetics and thermodynamics,^{5,6} demonstrations of kinetics,⁷ and exploratory data analysis.⁸

In this paper, we describe some of the Java applets we have developed and used in teaching introductory chemistry. In the following sections, we give a tour of some of our applets, and discuss their design, and their uses in lecture and homework. For each applet, we'll highlight the motivation for the topics or contexts we have selected and address questions such as:

- What are the primary advantages to teaching this material via simulation?
- How does the simulation improve the learning process (e.g. aiding visualization, providing scaffolding to reduce floundering)

- How does the simulation enhance students' interest in the material? (e.g. providing meaningful contexts, increasing interactivity)

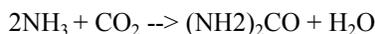
This paper is a progress report and current thoughts on our work in progress as well as our preliminary experience with using the software in introductory chemistry at Carnegie Mellon (<http://ir.chem.cmu.edu/chem106/>). We will present a number of Java applets that illustrate various uses and design approaches. We will close by discussing our plan for integrating these approaches, and present a proposed development environment to maximize the benefits of simulations in curriculum development.

Visualization to get beyond recipes: Stoichiometry

The goal of this applet is to get students to see beyond the recipe for solving limiting reagent problems. The students often learn this as a stepwise procedure. In the initial stages of learning, students will often have correct intermediate results written down but not understand what these really represent and so are not able to complete the problem. Even once they learn the procedure, without deeper understanding, retention is bound to suffer.

The applet can be found at (<http://ir.chem.cmu.edu/irProject/applets/stoich/> and click on "applet") Consider using the applet while solving the following problem, Example 4.5 of Chang:⁹

Urea [(NH₂)₂CO] is used as fertilizer and as animal feed and is used in the polymer industry. It is prepared by the reaction between ammonia and carbon dioxide:



In one process, 637.2g of NH₃ are allowed to react with 1142 g of CO₂. (a) Which of the two reactants is the limiting reagent? (b) Calculate the mass of (NH₂)₂CO formed. (c) How much of the excess reagent (in grams) is left at the end of the reaction?

By clicking on the bars in the upper panel, the initial grams of the reactants may be entered. As the slider bar is moved to the right, the bar-chart shows that the moles of NH₃ decrease twice as fast as those of CO₂, giving a visible image of the meaning of the stoichiometric coefficients. Pulling the slider bar across the screen shows the reactants disappearing and products appearing. When the slider is positioned all the way to the right, the reaction is complete and it is clear that the reaction has ended because the NH₃ has run out. The applet thus provides a visual image of the limiting reagent calculation which may be useful both in lecture and during homework.

The limiting reagent applet is meant for reactions that go to completion. An extension of this applet builds in the idea that the equilibrium position of a reaction is set by the equilibrium constant. (<http://ir.chem.cmu.edu/irProject/applets/equilib/>) In this applet a dot has been added to the slider to indicate the equilibrium position of the reaction. The common visual theme will encourage students to make connections between this new

material and that covered a few months previously, possibly even by a different instructor in the first semester of a two-semester introductory course.

Uses in Lecture

The lecturer can begin by using the applet to illustrate the concept of a limiting reagent in a detailed and concrete manner without the need to perform any explicit mathematical calculations. He or she may then work through the calculation on the blackboard while referring to the applet to illustrate what is being calculated and why. The conversion from grams to moles can be motivated by using the applet to stress that it is the moles of the reagents that change in a manner that can be easily derived from the stoichiometric coefficients. After calculating a number on the blackboard, the lecturer can pull the progress bar to the relevant position and illustrate what has just been calculated so that students can see how that number fits into the overall scheme. Finally, the conclusion of which reagent is limiting and how much of each product is produced can be confirmed. Throughout, the applet serves as a constant reminder of what is being calculated and why.

Note that the applet provides an alternative representation that complements what is usually presented on the board. It does not approach or solve the problem as it would be done with paper and pencil. Rather, it serves as a supplement to such calculations, with the goal of providing students deeper insight into the qualitative nature of the system and the calculation. While the specific approach to calculations varies between textbooks and faculty members, our goal is to “simulate” the system in a manner that can accommodate any correct approach.

Uses outside the classroom

Students can use the applet while performing practice problems. It can be used to check their answers and, when they disagree, provide an instrument for them to discover and correct their own errors. For instance, if a problem involves a number of intermediate steps, students can check these intermediate steps. If a student begins doing manipulations and gets confused as to what it is they are calculating, comparing their numbers to those on the applet may help bring the student back on track. For instance, the introduction of an intermediate variable representing the number of moles consumed is not explicitly included in the applet.

Visualization of complex phenomena: Color

This applet illustrates the use of a simulation to allow students to focus on different components of a complex phenomenon like why things have color (<http://ir.chem.cmu.edu/irProject/applets/color/>). We chose this topic because the particle in a box is potentially exciting but this excitement often gets derailed in the mathematics. A complete understanding of this phenomenon requires students to first understand a number of different concepts and then assimilate them into an integrated whole. This is especially true of its use in lecture. Achieving this goal requires students' attention to be directed to, for example, how changing the parameters of the particle in a

box changes the color absorbed by the material. This applet is meant for use as a lecture tool before it is used to contextualize homework problems.

Uses in lecture

The following is a sample lecture outline using the color applet:

Light is composed of colors that can be dispersed and recombined with a prism.

A substance that absorbs a certain color appears to have the complementary color. (This may be demonstrated by adjusting the parameters of the particle in the box to get it to absorb the desired color. At this point, no mention of the particle in the box should be made beyond saying that the material is being altered so that it will absorb the desired color.)

The absorbed photons have an energy that corresponds to the spacing between quantum energy levels. The applet may be used while discussing the existence of energy levels. It can also be used to demonstrate that it is the difference between the energy levels that determines the color of light absorbed.

The qualitative aspects of the particle in a box model may then be discussed, focusing on the fact that a particle confined to some region of space will have discrete energy levels. General features of the dependence on mass and length can then be discussed. One suggestion is to create a table on the chalkboard of the spacings that result for some representative lengths and masses. These tables may then be referred to in the later mathematical discussion.

The visible spectrum is a small portion of the electromagnetic spectrum. This can be demonstrated using the full spectrum at the top of the applet, and showing that it is only for a small range of box sizes that an electron will absorb visible light.

The previous topic leads nicely into a discussion of **what molecular motions lead to absorption in what part of the spectrum.** For instance, the idea that an electron has to be in a fairly large box can be used to rationalize why many dyes are conjugated organic molecules. The length of a standard chemical bond can then be discussed and the applet used to demonstrate that an electron in a typical bond absorbs light in the UV. It can then be pointed out that electrons are not the only particles that move in a molecule. By putting a particle with a mass of a few amu's (ex. 5) in a box of a few tenths of an angstrom (ex. 0.3A), it can be shown that molecular vibrations tend to lie in the infrared. Rotations can be discussed as confining the nuclei to a ring with a circumference of 10's of angstroms, and the applet used to show that such rotations lie in the microwave region. The calculated quantities may be added to the chalkboard table of parameters and calculated quantities started above.

As in the previous stoichiometry applets, this applet enables a fairly thorough and concrete discussion of what phenomena the particle in a box model can be used to explain. Once students know why they should be interested in the model, the mathematics can be discussed on the board. In the above lecture the results obtained while using the applet were written on the board. These results may now be explicitly calculated while going back to the applet to remind students why that particular example was of interest. For instance, if it was calculated to show that electrons in normal bonds absorb light in the UV, then that point can be reinforced and students reminded of the goal of the mathematical calculation.

Uses outside the classroom

The applet can be used both to allow students to answer qualitative questions, and to allow students to check their paper-and-pencil calculations. For instance,

Students can be given the typical size of a nucleus and asked to use the applet to determine the photon energy associated with excitations of the motion of a proton inside a nucleus. This illustrates the wide range of phenomena that can be qualitatively understood with this simple model.

Another suggested qualitative problem is to explain to students that “electrons” in a semiconductor have effective masses that differ from that of a real electron. The use of quantum well devices can then be explained and students asked to determine the size of a layer needed to have energy level spacings in the red. A more interesting way to phrase the question is in terms of how many atoms thick a layer would need to be for a quantum-well laser to emit photons in the red.

If students are asked to solve particle in a box questions with paper and pencil, the applet can be used to check their final answers. Note that the applet does not do the work for them. It is roughly equivalent to providing the numerical answer to a practice question, such as is often done at the end of a textbook.

Homework as an Inroad

Our primary inroad to improving student learning is through the course homework. We have chosen to focus on homework rather than lectures or laboratories for a number of reasons.

- First, it is in the active processing of the information that most learning occurs, and the most effective processing occurs when students are applying concepts in solving problems, either during homework or while studying for exams.
- Second, interactive simulations have the potential to better utilize student’s time by providing meaningful feedback and scaffolding, preventing them from either floundering or reinforcing incorrect thinking.
- Third, current homework is perhaps the least motivating portion of the course for students.
- Fourth, assigning a new style of homework problem is an easily implemented step towards improving a course, and involves relatively low risk, especially if first done as bonus or optional homework.

While lecturing brilliantly on how a chemical topic relates to an interesting real-world phenomena can excite students, such excitement is bound to fade if the homework does not sustain this interest. We believe that homework that reinforces this connection is essential if such teaching innovations are to lead beyond motivation to enhanced learning. This is what motivated us to develop the following applets which focus on using simulations to improve homework.

Interacting with complex phenomena: Everest

This applet (<http://ir.chem.cmu.edu/irProject/applets/everest/>) is meant to add relevance to the equilibrium portion of the course and provide an interesting problem solving activity. The Everest context provides a familiar, real-world context which motivates

students and a goal that requires a fairly deep understanding of equilibrium. The primary use of this applet is as a automatically grade homework assignments. Students receive a handout describing the chemical equilibria involved and their goal, to the top of the mountain before winter hits and without passing out due to lack of oxygen.

With the color applet we addressed the use of the simulation as a way of drawing students' attention to different features of a complex phenomenon. The Everest applet allows students to interact with one component of an complex phenomenon. Since almost every real-world example has many integrated concepts, this benefit of simulation-based homework is especially important. For instance, many applications, including this one, involve time dependencies that are well beyond introductory courses. Here it is in the body's growth of hemoglobin in response to high altitude. The kinetics of this are handled by the computer in a manner that does not confuse or distract the student.

To start the applet, click on Base Camp in the trail map. As you rest as base camp, your body grows hemoglobin. The student's job is to figure out how long they need to rest to have sufficient hemoglobin to survive at the next camp. If they rest too long, winter hits before they reach the top. If a student reaches the top, e-mail is sent to a course account so that he or she receives appropriate credit.

Uses outside the classroom

This problem has been assigned to students in our introductory course as a bonus problem. The students' response was positive and gave a good indication that we achieved our motivational goal. However, our initial learning goal was to teach them to derive an equation relating the necessary amount of Hemoglobin to the partial pressure of oxygen. This was not as successful. It appears that most students solved the problem by trial and error. But since many used rather sophisticated guessing strategies such as linear interpolation schemes, we are still deciding whether we should limit the number of attempts allowed in order to prevent trial and error approaches in the future.

Doing homework in learning environments: Virtual Lab

Our most well-developed applet to date is a Virtual Lab which handles all of the aqueous reaction types and thermodynamics commonly covered in introductory chemistry (<http://ir.chem.cmu.edu/irProject/applets/virtuallab/>). Users can select from hundreds of standard chemical reagents and mix them together in any way they see fit using equipment and procedures commonly available in introductory laboratories. This software differs from the previously described applets in that it is both general and flexible, so that it can be easily incorporated into existing courses at diverse institutions and may be used to meet diverse goals. For example, some instructors may want to focus on reducing students' difficulty in making connections between theoretical concepts about the molecular level and observations at the macroscopic level, especially when both the concepts are observations are unfamiliar to the students. In those cases, providing practice with a simulation can increase familiarity with some observations and

begin to bridge the gap to theory. Some instructors may want to convey a greater intuition about chemical processes and wish to communicate more clearly the abstractions that are not immediately obvious from either manipulating chemicals in a physical laboratory or solving mathematical equations. Our hypothesis with the Virtual Lab applet is that we can speed the communication of this vision by providing students with a flexible environment where they can interact freely with chemicals and see directly how their actions modify the chemical species in solution.

One key feature for teaching complex concepts seems to be providing multiple representations so that students can flexibly encode and use what they have learned.¹⁰ Our software shows both a bench-top view of the experiment as well as a graphical representation of the species in solution so that students can immediately see the molecular-level changes in a reaction. The additional representations of the species in solution provide a small amount of scaffolding to enable students to detect errors when they occur, but otherwise the student's observations and feedback in this computer-based context are reasonably similar to a real laboratory experience. This type of technological support can facilitate students' perception of critical features to be learned.¹³ We are about to begin careful observations of student interactions with the software to see how effectively they are able to interpret this feedback in light of their hypotheses, since some research has shown that this connection can be difficult to make.

A primary goal of the applet was to create a student-centered educational environment in which students are given more meaningful goals and allowed a greater flexibility in achieving these goals. Because our simulation environment opens up a wider range of goals than paper-and-pencil tasks, alternative types of assignments can engage students' curiosity, provide a challenge, and allow students to make choices about the procedures they use.¹¹ For instance, the standard problem type of "A was mixed with B, calculate the outcome" can be transformed into "You want this outcome, what do you do to get it?". The latter resembles more authentic activities performed by chemists. Such goals have been suggested as a means to promote intrinsic motivation, and have the potential to increase students' time exploring chemical concepts and interest in pursuing the field as a career.

The Virtual Lab display is divided into the following three panels:

Stockroom Explorer This provides access to the chemistry stockroom.

Workbench This allows the user to perform chemical manipulations on the solutions. You can switch between workbenches by clicking on the tabs.

Solution Info Panel This panel displays information about the workbench's currently selected solution. The text lists the concentrations of the species in solution, in moles/liter. The bar chart shows the \log_{10} of these concentrations. The lowest panel is a pH meter.

Double-click a solution in the Stockroom bring it onto the workbench. To transfer liquid between flasks, drag the source flask onto the recipient flask. (The mouse pointer must be on top of the recipient flask, such that the recipient flask becomes highlighted.) The

source flask should appear rotated and above the recipient flask. You can now type the number of ml to transfer into the text box at the bottom of the screen and hit return or the pour button. Extra glassware can be retrieved using the buttons on the left of the workbench.

Uses in Lecture

Instructors can use the Virtual Lab in lecture to demonstrate phenomena such as titration curves and to promote a more intuitive understanding of pH and buffer zones. The Solution Viewer provides graphical reinforcement of the changing concentration of species in solution, while a pH meter enables students to follow the rate of change of pH with slow addition of base in a titration. While the lecturer must carefully narrate what feature to observe as the titration progresses, the multiple representations available to students may encourage deeper understanding of acid-base chemistry.

Uses Outside the Classroom

The Virtual Lab's design has as a core precept that what students practice is largely what they learn and retain.¹² A simple initial use of the Virtual Lab is to encourage students to check their understanding of textbook-style homework. Because they can check partial solutions to problems, many students will be able to avoid the frustration that comes with pursuing incorrect paths and to avoid reinforcing misconceptions by repeating them. A homework assignment, used this semester, that implemented this approach with regards to acid base chemistry can be found at <http://ir.chem.cmu.edu/chem106/assignments/hw5.pdf>.

We also intend this software as a tool to enable faculty to create a variety of assignments that promote stronger connections between chemical processes and pencil-and-paper calculations. Our approach is similar to other technology-enhanced student-centered learning environments¹³ which seek to actively engage students in constructing connections between new knowledge and existing conceptions and immerse them in concrete experiences to anchor their understanding, while also allowing the student freedom to explore. For example, some of these assignments may focus on practicing, planning and implementing, in a simulation environment, some procedures similar to what they would do as preparation for traditional laboratories. Some may focus on a “design” goal such as creating a buffer that would withstand the addition of a particular volume of acid. Others might be to design an experiment to address a particular question.

Consider, for instance, a student using the simulator to experiment with strong acids and bases. When a student adds NaOH to water, they will see immediately via a bar graph that it exists in solution as Na^+ and OH^- . They can then see that the primary effect of adding HCl is to consume some of the OH^- . Our hypothesis is that this interaction will give them a more intuitive feel for the reactions of strong acids and bases than could be imparted by listening to descriptions of the phenomenon in lecture or solving the related paper and pencil problems. Such visualizations become even more powerful when applied to more complicated phenomena such as the behavior of buffers.

A simple assignment, where students use the virtual lab to measure the binding constants between nucleic acids, can be found at <http://ir.chem.cmu.edu/chem106/assignments/bonus1.pdf>. A more challenging assignment, in which students must first characterize a weak-acid dye and the binding of this dye to DNA and then construct a buffer to achieve a certain percent binding, is located at <http://ir.chem.cmu.edu/chem106/assignments/hw-bonus2.pdf>.

Future changes

Due to popular demand, we need some things that blow up. In addition to expanding the range of chemical phenomena that are included in the simulation, we are working on functionality that will aid in creating interesting problems. Many of these functionalities involve restricting what features are available to students. For example, to allow identification of unknowns, it will be necessary to turn off the bar chart showing the species in solution. Turning off the pH meter will be useful for problems involving indicators for titrations. We are also adding ability for problems to be automatically graded.

Pulling it all together: Real-world phenomena using Virtual Lab

We are currently developing a system to allow easy development of real-world problems that utilize the Virtual Lab. For instance, in our Virus Sniffer (currently under construction), students can explore an island looking for biological weapons facilities. In the process they will come across solutions which they must take to the Virtual Lab and analyze. They will also create solutions for use on the island. Hopefully, some problem utilizing using this new curriculum construction tool will be available at the time of this conference.

Summary and Discussion

Based on our experience developing and testing this series of applets in a preliminary way, we have converged on some overall strategies for using simulations:

- Simulations help in lecture to keep students focused on the overall goal and qualitative issues and to prevent the chemically significant concepts from getting lost in calculations (as in the stoichiometry and color applets).
- Simulations allow students to see concepts in meaningful contexts, thus providing motivation for the more abstract and complex material in introductory courses (as in the color and Everest applets).
- Simulations enable students to first focus on each separate aspects of a complex phenomena, and then later assimilate these into an overall understanding (as in the color applet with delayed introduction to particle in a box).
- Simulations allow students to interact with selected parts of a complex phenomena, while the computer handles those skills that are beyond the current level of the student (as in Everest).

- Concept reinforcement and transfer between various portions of the course can be promoted by using a common simulation (such as the Virtual Lab), but allowing students to interact with different components at different times throughout the course.

As discussed in Section ?, Homework based on simulations can provide an ideal inroad to improving large lecture courses (as in both Everest and the Virtual Lab). It also may have a number of significant advantages over the most closely corresponding paper-and-pencil activities, as shown in the following table.

Challenges with traditional homework	Benefits of Simulation
Classic textbook problems may inadvertently overemphasize quantitative reasoning over qualitative and conceptual reasoning.	Simulations can focus students on observing and predicting key phenomena based on fundamental concepts, while potentially extending learning from calculation-based problems.
Introductory course material makes it difficult to develop problems involving more than a single step, and most real-world phenomena involve multiple concepts and time-dependence.	Simulations allow the computer to handle the topics that students aren't ready for, and allow students to interact with just that portion they are currently studying.
Achieving realism often requires a complex cover story, but often the story can be ignored in solving the single-step problem embedded in it.	Allowing students to interact with different portions of the simulation at different points in the course may help them deal with realistic phenomena and integrate the material from different parts of the course in a meaningful context. This benefit can be extended to cross-discipline simulations.

Our vision for the next stage in developing software for introductory chemistry that maximizes the learning benefits of simulations for a large number of students includes the following design principles:

- The software should be both general and flexible so that it can be easily incorporated into existing lectures and laboratories at diverse institutions. For instance, the Virtual Lab software can be used in a variety of ways to fit the educational goals and environment of a specific course and institution while remaining easy to work with for faculty who do not want to spend time programming.
- The software should complement rather than attempt to replace the primary teaching materials in the course. While multi-day modules allow for deep exploratory

learning, smaller components are more easily integrated into courses with hundreds or thousands of students.

- The software should empower large numbers of faculty by giving them tools to develop new teaching methods via low-risk incremental changes. Taking a curriculum development strategy which combines course modules¹⁴ or applets on specific topics,¹⁵ with a general laboratory simulation invites faculty to reflect on both broad course goals, such as teaching students to reason scientifically, and specific content, such as the behavior of weak acids and bases.
- The design of the software should draw on teaching and learning research, such as that in technology-enhanced learning environments,¹⁶ inquiry or discovery learning,¹⁷ skill acquisition,¹⁸ and motivation theory.¹⁹ For instance, a core principle guiding our work is that to improve students' conceptual understanding we must substantially change how students interact with the material and better facilitate their exploration of relationships between abstract theoretical concepts and observable chemical processes.
- The technical implementation of the software should be easy to deploy in a complex heterogeneous computing environments and minimize the logistics that can be especially time-consuming in large courses. Network computing technologies such as the Java computing language and networked databases have been used successfully in corporate information systems to tackle similar challenges. Our goal is to allow our software to be run from any computer with an Internet connection and a Java-enabled browser; however, the Virtual Lab uses Java-2 which currently requires that the user take the time to download the Java plug-in.
- Finally, a practical feature of simulations that can have a substantial educational impact is integrating the software with the course structure and management so that it can be adopted in many courses. Since developing new assignments creates new grading demands and often requires the creation of new grading criteria, software must be able to support these important evaluation and feedback activities in order to be used widely. We are currently working on integrating our software with a database that collects assessment data on student activities and allows automatic grading of student assignments.

Acknowledgements

This work was funded by the National Science Foundation, Division of Undergraduate Education, Award 9950673.

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