ChemLogo: An emergent modeling environment for teaching and learning chemistry

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Abstract: The aim of this paper is to explore the potential impact of a novel modeling and simulation package, ChemLogo, on students understanding of chemistry. ChemLogo is embedded in the NetLogo modeling environment and teaches chemistry from the perspective of emergent phenomena, that is, macro-level patterns in chemistry result from the interactions of many molecules on a micro- and submicro-level. In this paper, we examine student understanding of chemical equilibrium and problem solving with and without ChemLogo. A three-part, 90-minute interview was administered to six undergraduate science majors. Several common misconceptions about chemical equilibrium and ineffective problem solving techniques emerged during the interview. Prior to their interaction with ChemLogo, students relied on rote memorization and application of rigid algorithms to solve chemical equilibrium problems. Using ChemLogo students employed problem solving techniques characterized by stronger attempts at conceptual understanding and sense-making, using micro-level interactions to give causal accounts of macro-level phenomena.

1.0 Introduction

Many students view chemistry as one of the most difficult subjects to study. Learning chemistry places many demands on students and teachers that can seem insurmountable. Instructors often display mathematical formulas, chemical symbols and scientific measurements simultaneously to describe phenomena that are not visible to the student. Moreover, the "abstract" concepts of chemistry are often seen as confined to the chemistry classroom and not applicable outside of school. To deal with such difficulties, chemistry educators have devoted considerable time to developing curricula that help students visualize the molecular world and connect classroom concepts to the world outside of school. In particular, a few novel curricula employ computer-based learning environments as visualization tools with which students reason

about chemistry. Following on these previous efforts, this paper introduces a new computer-based modeling environment for learning chemistry. The learning environment, ChemLogo, not only supports students' visualization of the molecular world, but also provides them with the opportunity to interact with and to manipulate the simulated world to gain a deeper understanding of core chemistry concepts and phenomena. In this paper, we present some findings on the use of ChemLogo to learn about chemical equilibrium.

2.0 Conceptual Difficulties in Chemistry Education

Considerable research has been devoted to identifying and classifying student misconceptions about chemical equilibrium (Quílez-Pardo & Solaz-Portolés, 1995; Tyson & Treagust, 1999). Recently, researchers have also begun to explore pedagogical difficulties with the representation of chemical phenomena on multiple levels and the forms chemists give those representations. Experienced chemists take for granted that chemical phenomena occur on many levels (Johnstone, 1993). Due to the submicroscopic level of molecular interactions, chemists must use symbols to refer to the atomic objects and processes within their domain which they cannot observe directly. Moreover, aggregations of molecules result in phenomena on a macroscopic level such as when water freezes or ice melts. On the symbolic level, where most teaching and learning take place in the traditional chemistry classroom, instructors use multiple representations for the same phenomena (Kozma & Russell, 1997). A particular chemical reaction may be represented on the blackboard with letters, molecular diagrams, or plots of concentration over time. In the laboratory, students are further expected to connect the symbolic representations in texts to the actual physical substances they use in an experiment and the numerical measurements they take from laboratory instruments. Although chemists may easily discern the relationships between chemical phenomena at the submicroscopic, microscopic and macroscopic levels and fluidly move between various symbolic representations of the phenomena, students have considerably more difficulty (Banerjee, 1995).

One design approach that has enjoyed much recent success in directly addressing the conceptual difficulties of chemical equilibrium utilizes computer simulations of chemical reactions to highlight the relationships between the various representations and levels. These curricula take an inquiry-based approach to teaching chemistry. The inquiry approach has been successful in many science domains, and many chemistry educators now advocate for its use in the chemistry classroom (Barowy & Roberts, 1999; Bodner, 1992). Curricula of this nature provide students with a learning environment in which they can study a concept as it relates to a particular system, make predictions about that system, and justify their predictions with observable outcomes. This approach discourages rote memorization and formulaic problem solving, while encouraging conceptual understanding and critical thinking.

In the chemistry classroom, computer-based inquiry attempts to make explicit the information embedded in traditional molecular representations as well as to provide a visual representation of molecular interactions that students can manipulate. Such software provide the student with "multiple, linked representations" that foster conceptual understanding and emphasize the connections between representations to aid problem solving (Kozma, Russell, Jones, Marx, & Davis, 1996, p. 41). Here, students learn chemistry by viewing molecular animations side-by-side with graphical outputs and chemical formulas. Because students can modify system variables of the chemical reaction under study, they can make predictions based on their understanding of relevant chemistry concepts. Consequently, students can monitor their learning by observing the results of their interactions with the system.

2.1 Teaching Chemistry Concepts as Emergent Phenomena

Though such chemistry computer-based learning environments have resulted in improved student

understanding, much of the current software is "first generation" and is limited in its approach to teaching chemistry. A significant limitation is that many of the simulation packages currently available are designed as "black-boxes". The simulations are programmed with a specific number of activities and learning outcomes for students and teachers. Students are given a limited number of variables that can only be manipulated in predefined ways. Moreover, the molecular visualizations that give students access to submicroscopic interactions between molecules are often delivered as simple animations: for each set of variables that a student selects, one particular animation is displayed. These qualities both reduce the software's effectiveness as simulations of actual chemical phenomena and limit their use as inquiry tools in which students can make novel hypotheses and explore outcomes.

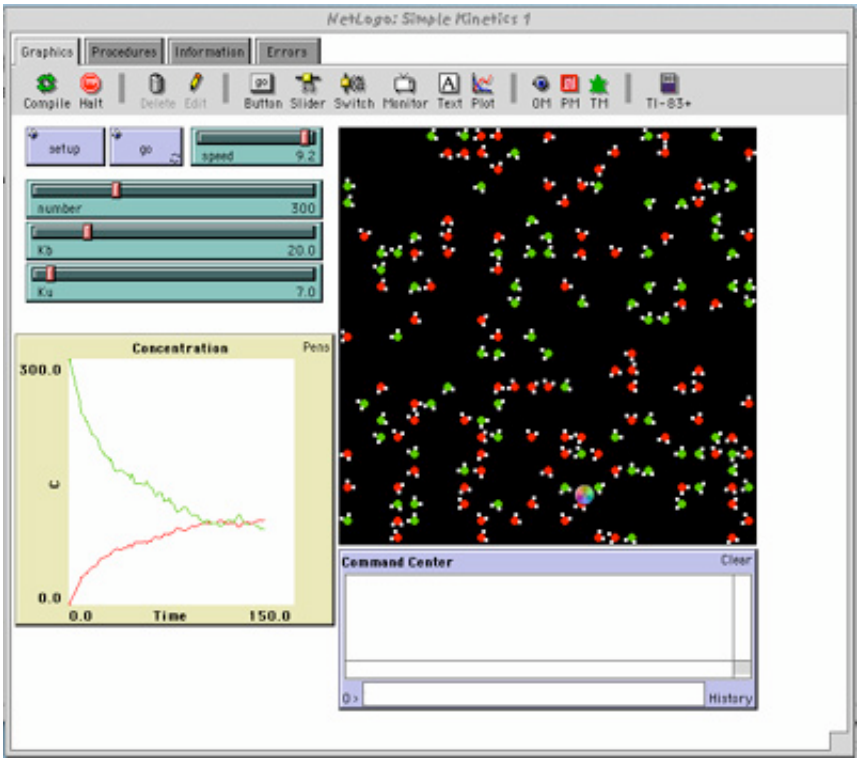
To overcome these limitations, we suggest that a better approach to the design of computer-based learning environments for chemistry rests on the idea of teaching chemistry from the perspective of emergent phenomena. The concept of emergent phenomena recognizes that patterns observed on the macro-level "emerge" from the interactions between many agents on a micro-level according to specific rules that govern individual agents' behavior (Wilensky, 2000). For instance, the specific interactions between billions of molecules in a glass of water can result in a liquid, a solid block of ice, or a cloud of steam. By giving students access to the rules that govern the individual behavior of molecules, students can visualize and explore how chemistry theories and concepts emerge from molecular interactions on the submicroscopic level. Traditional curricular approaches ignore the connection between levels, which leaves students with little recourse but to memorize macro- level patterns without tying them to molecular interactions. Consequently, students frequently apply incorrect concepts and misremembered facts during problem solving. By providing students with an environment in which they can learn how molecular interactions result in specific chemistry patterns and concepts, we can expect to enrich their understanding and increase their ability to solve novel problems. By engaging in model-based inquiry, students are able to reason more effectively across levels instead of struggling to remember algorithms and rote facts. To this end we have developed ChemLogo, a computer-based learning environment, to teach a variety of chemistry concepts in both secondary and undergraduate classrooms.

3.0 The Learning Environment: ChemLogo

ChemLogo consists of a number of particular computer-based models written in the multi-agent modeling languages (MAML) StarLogoT (Wilensky, 1997) and NetLogo (Wilensky, 1999b). MAMLs have been employed in a variety of biology (Wilensky & Reisman, 1998) and physics (Wilensky, 1999a; Wilensky, Hazzard & Froemke, 1999) classrooms to help students understand how micro-level interactions between individual agents can result in observable patterns at the macro-level. Frequently, in a traditional classroom, these observable patterns are taught as isolated concepts and laws that students are required to memorize. In a MAML environment, students come to understand these concepts and laws through a process of exploration and inquiry — by investigating and controlling the behavior of thousands of graphical "agents". By interactively exploring the relationship between the agents' rules of behavior and the patterns that emerge as a result of these rules, students are able to "debug" misconceptions that are generated by confusing their understandings of micro- and macro-level interactions. Typically, in curricula using multi-agent modeling, students begin by exploring the behavior of pre-built simulations designed to focus on some target concepts. They make predictions about the behavior of the model under varying model parameters then test their predictions by exploring model outcomes as they change 'sliders' in a simple graphical user interface. Students, however, may at any time open up the black box of the interface and examine (or change) the underlying rules that animate the individual elements of the model. The ChemLogo package consists of several such pre-built models designed for teaching target chemical concepts. Each of the models

simulates a closed chemical system that students can interact with in several different ways.

The core of every ChemLogo model is the *interface window*. Typically, the interface contains a graphics window, a plotting window and several variables in the form of sliders and buttons that the student can manipulate. It is here that students can observe directly the interaction between the micro- and macro-levels. For instance, in the "Simple Kinetics 1" (Figure 1) students can observe in the graphics window how a collision between two nitrogen dioxide molecules can result in the formation of one dinitrogen tetroxide molecule. As a result, the macro-level concentrations of each chemical species change as reactions occur. By manipulating the sliders for predefined system variables, students can observe how varying the reaction rate constants alters molecular behavior and consequently the concentration plot. ChemLogo models are not limited to the predefined variables of the software designers, however. The models are easily modifiable and students can add or remove variables from the interface window to explore thoroughly the behavior of a reaction.



(click image to enlarge)

Figure 1. The ChemLogo interface window contains a graphics display, plot output and system variables.

A critical advantage of ChemLogo over other computer-based inquiry environments is that each model is built as a "glass-box". Students can manipulate not only the variables that are provided in the *interface window* (Figure 1); in the *procedures window* they can also alter the NetLogo code that governs molecular behavior (Figure 2). The NetLogo code is user-friendly and the ChemLogo materials encourage instructors and students to modify procedures and observe how the chemical system is affected. For example, students might alter the procedures to introduce a catalyst into a model and observe how the reaction changes. A detailed description of the chemistry concepts underlying the model and suggested extensions of the procedures accompanies each model in the *information window* (Figure 2). The design of ChemLogo enables students to explore concepts outside the initial boundaries of each model. Thus, students' spontaneous questions and novel problems can easily be addressed as they occur in the classroom. Together

the procedures window, the interface window and the information window draw together the micro-, macro- and symbolic levels of chemistry so that students are not forced to rely on only one level. For example, in the model "Simple Kinetics 1", students can observe in the information and procedures windows how molecular behavior is characterized by discrete mathematical relationships and why specific variables such as temperature and pressure can influence the outcome of a chemical reaction. They can modify any variables and see how the consequences of their modifications in the interface window.



(click image to enlarge)

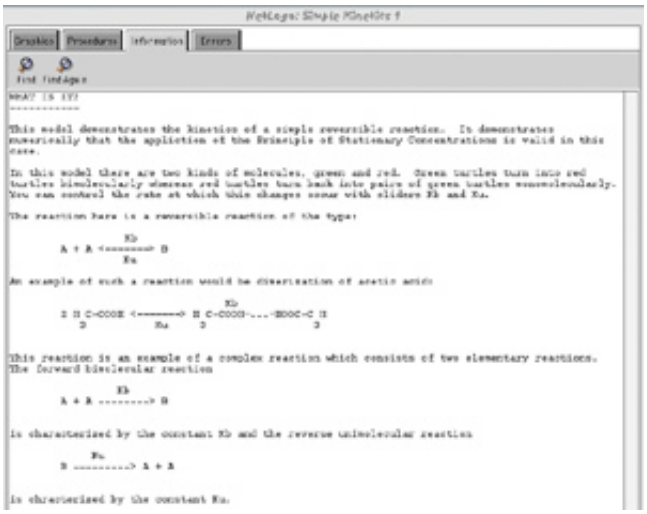


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Figure 2. Connections drawn between the model procedures and information windows together with the interface window help to enhance students' conceptual understanding on the symbolic and submicroscopic levels.

4.0 Exploring the Potential Benefits of ChemLogo?

To explore the effectiveness of the ChemLogo modeling environment for facilitating students' exploration and understanding of chemical equilibrium, we conducted a small study with six advanced undergraduates at a large research university. Though ChemLogo was designed for use in an introductory chemistry course, we felt that we could explore some of the potential benefits of the software by observing the interactions of students already familiar with the concept of chemical equilibrium to identify particular areas where the model is most and least effective. Each of the students interviewed in this study was self-described as high achieving in the sciences, particularly chemistry and biology, and each intended to pursue careers in science or medicine. All six of the students reported originally learning about chemical equilibrium in introductory high school chemistry and that they had not covered the concept again explicitly in any of their higher-level chemistry courses.

4.1 Why Model Chemical Equilibrium?

The concept of chemical equilibrium (and its' related ideas) is frequently introduced to students in a high school general chemistry course, where it is often the first and last course in which the concept is directly addressed (Voska & Heikkinen, 2000). Though chemical equilibrium is rarely taught explicitly in higher-level courses, it is a recurrent concept that is vital to understanding many chemical processes. At its most basic level, the concept of chemical equilibrium requires that students understand the relationships between

several physical variables (e.g. pressure, temperature, concentration), several mathematical and symbolic expressions (e.g. reaction quotient, equilibrium constant, rate law), and the equilibrium position (i.e. the relative ratio of reactants and products) of a chemical reaction. Typically, students learn the concept of equilibrium by memorizing a definition and a list of rules for predicting the equilibrium position of the reaction based on the reaction variables (Tyson & Treagust, 1999). As with many other scientific concepts, the traditional emphasis on rote memorization and algorithmic problem solving often results in poor understanding, retention and application of chemical equilibrium concepts (Quílez-Pardo & Solaz-Portolés, 1995). Because of the difficulty students have in mastering the concept, there is a critical need for the development of improved methods and materials that facilitate a better understanding of chemical equilibrium.

4.2 Interview Protocol?

The protocol for the study consisted of three separate parts in a 90-minute interview (see Table 1). The first portion of the interview aimed to uncover each participant's recall and understanding of chemical equilibrium. For this, participants were asked various questions that allowed them to explain, in their own words, chemical equilibrium and any information they felt was important to the concept. The second portion of the interview attempted to discover each participant's ability to apply chemical equilibrium concepts to traditional textbook questions. The final portion of the interview protocol required students to make predictions about the equilibrium state and position of a particular reaction, $\mathbf{2NO_2 \leftarrow \rightarrow N_2O_4}$, which they then verified using the ChemLogo model, "Chemical Equilibrium 1". For each question, participants were given an initial set of conditions for the system followed by a final set of conditions in which one or two variables were changed while the others remained constant. Typically, the simulation was first run using the set of initial conditions and participants would observe the molecular interactions. The interviewer would then pose a question about the behavior of the reaction and the participants would make their predictions. The participants then modified the simulation, after which they would explain their observations of the system and compare them with their initial predictions.

Table 1. Format of Protocol Questions

Interview Level	Example Questions
Recall and Explain Chemical Equilibrium	"Define chemical equilibrium" "State factors that can affect reaction equilibrium
Traditional Problem Solving	$Ag_2CO_3(aq) + 2HCl(aq) <---> 2AgCl(s) + H_2CO_3(aq)$ Do the states of each of these substances have any bearing on the equilibrium position of the reaction?
ChemLogo Problem Solving	Chemical Equilibrium 1 models $2NO_2$ (g) <---> N_2O_4 (g)

	Can you tell by looking at the graphics window only if the system is in equilibrium? " "What else would you need to know?" "What will happen if you decrease the volume of the container?…You decreased it, what happened to the system? Is this what you predicted?"

5.0 Results

Observing the participants' interactions with ChemLogo revealed a number of common misconceptions about chemical equilibrium. Though these misconceptions served as a point of reference from which we observed changes in student thinking and problem solving, we will not list them as they have been reported at length elsewhere (Banerjee, 1991; Quílez-Pardo & Solaz-Portolés, 1995). Rather, our observations of student thinking over the course of the interview, most notably during the use of ChemLogo, centered on a dramatic change in conception, articulation, and application of the concepts underlying chemical equilibrium. Most important, we observed that the participants' dependence on formulaic problem-solving approaches and rote memorization at the start of the interview gave way to more thorough attempts at conceptual reasoning and justification of answers during their use of ChemLogo — a desired result of inquiry-based curricula (Barowy & Roberts, 1999). Such changes in student thinking were especially salient in four distinct categories: (1) defining equilibrium for a chemical system, (2) characterizing factors affecting equilibrium, (3) transitioning between submicro-, micro-, and macro- levels during problem solving and (4) fluidly moving between various forms of symbolic representation at all three phenomenal levels. Here, we elaborate on the evolution of one participant's definition and conceptual understanding of chemical equilibrium.

5.1 Equilibrating the Concept of Equilibrium

Difficulty in defining equilibrium is often found among chemistry and biology students when students misconceive of equilibrium as a static process (Banerjee, 1991). When a chemical reaction is in equilibrium, the rate of conversion of reactants to products is equal to the rate of conversion of products back into reactants. Thus, at equilibrium the relative concentrations of each molecular species remains constant on the macro-level; however, on the submicro-level, individual molecules are continually converted from reactant to product and back again. Chemical reactions do not stop when they are at equilibrium. Thus, equilibrium is dynamic process, which many students fail to see because of the stable macro-level concentrations of each molecular species. Surprisingly, the students involved in our study had no difficulty stating the dynamic nature of equilibrium at the beginning of the interview. When questioned initially, each participant reported that they had learned from texts that although the concentrations of chemical species remained apparently constant, reactions continued on the submicro-level when a system is at equilibrium.

Though at first it appeared that each of our participants possessed a stable, accurate definition of chemical equilibrium during the initial phase of the interview, inconsistencies in their conceptual understanding quickly became apparent when they were asked to describe the equilibrium state of specific chemical reactions. While answering several questions regarding the equilibrium state and how different variables would affect that equilibrium, the students all displayed difficulties. Their previously solid definitions and conceptualization of chemical equilibrium fluctuated to depend sometimes on rate and sometimes on

concentration. Their reasoning often failed to include vital characteristics of the chemical species in question, such as whether a product boiled out of solution as a vapor. Even when the interviewer pointed out these factors, the students were unable to incorporate the new information into their explanations. When the students were asked questions on traditional chemistry problems (without ChemLogo), it was evident that they were reasoning by rote recall. They almost unanimously justified their responses by stating the definition of equilibrium as told to them by previous instructors or textbooks though it was not an appropriate justification for many answers.

Over the course of the 40-minute interaction with ChemLogo, the transition in participants' thinking from a dependence on rote recall to conceptual reasoning became increasingly apparent. One participant, Andrew exemplifies this transition. Whereas Andrew initially relied almost exclusively on formulae and rote facts to answer questions about chemical equilibrium, his problem-solving techniques took on the more critical aspects of a scientific researcher while he was engaged with ChemLogo. When discussing his reasoning, Andrew was able to recognize and correct his own misconceptions about the definition of chemical equilibrium. By observing both how the interactions between molecules in the graphics window changed according to system variables and how the concentrations of each species changed in the plotting window, Andrew identified, evaluated, and refined his understanding. As in other inquiry-based curricula, Andrew's conceptual evolution was supported by the ChemLogo modeling environment: the model allowed him to make predictions and receive instant feedback as well as provided opportunities to validate and justify his answers by exploring alternative paths of reasoning.

The nature of Andrew's change in reasoning becomes clear over the course of the interview. As in the traditional problem solving session of the interview, he bases his answers during his first interaction with the ChemLogo model on the faulty recall of rote facts, but by the end of the interaction, he supplies more conceptually sound arguments for his answers. When first defining the equilibrium state, Andrew correctly states the definition of equilibrium but incorrectly states that the concentrations of products and reactants should be equal at equilibrium. After interacting with ChemLogo, he finds that the model's feedback contradicts his initial predictions. Subsequently, he begins to clarify whether it is rate or concentration that determines chemical equilibrium.

> **A**: Yeah, so the amount of red (N_2O_4) turning to green (NO_2) and the amount of green turning to red-that rate is equivalent-but somehow they're (the molecules) satisfied … that there is more green than there is red.
>
> **I**: So does that fit in with what you said earlier that we would make equal amounts…?
>
> **A**: No.
>
> **I**: Can you explain why that's happening?
>
> **A**: Um…Maybe it's because I overlooked the coefficient, you require two molecules of NO_2 to one N_2O_4. It's not a 1:1 ratio.
>
> **I**: Oh, so we would always have more greens than reds?
>
> **A**: Yes. Because you're going to need a lot more greens to make a red as opposed to the other way around. That's a basic concept I should've known.

Here, Andrew has used the model to refine his concept of equilibrium, but he still incorrectly predicts that there will always be more reactants than products. Andrew indicates that there will always be a greater number of green reactants because of their coefficients, which he bases on the fact that it requires two NO_2 molecules to form one N_2O_4 molecule. Here, he shows a dependence on the symbolic representation of the reaction for his explanation. ChemLogo's pedagogical benefits become more apparent as the interview proceeds.

A: …So now we have a lot more of this (green) to begin with. Well, I am going to see a similar trend, but up here (points to the top of the y axis)…I'm wondering what will happen to the red, will it increase, but I don't think so. Should I press run?

I: Go ahead… So, you looked surprised, we've got more reds than greens.

A: Yeah, I was afraid that was going to happen. (Laughs)

I: Does that make any sense? Would you say they are at equilibrium?

A: Yeah. So this obviously is what happens ideally. Like this is the correct way?

I: Yeah, no deception here.

A: Right. Based on that this tells me that what I said was wrong before. I can conclude from this that if you dump in a whole bunch of NO_2 then you're going to get an even higher proportion of N_2O_4, red, at a certain point. And you have so much more red that's going to dissociate back to green. But because you initially added so much green you caused an increase in red.

Because Andrew was able to use the software to test his predictions and receive immediate feedback, he was able to evaluate and modify his understanding. Rather then attempt to answer the interview questions based on rote recall, Andrew was able to think more critically about each problem to arrive at a more conceptually justified answer. In each instance, Andrew refers to the behavior of the molecules in the model to determine his final answer. The form of the feedback in ChemLogo is critical. In the plotting window, ChemLogo displays the relative concentrations of each molecular species on the macro-level, from which Andrew can confirm or reject his hypotheses and predictions by observing the reaction proceed in real time. Moreover, in the graphics window, ChemLogo supports Andrew's conceptual reasoning by displaying the submicro-level interactions between the reactants and the products. By observing the chemical phenomena on both levels simultaneously, Andrew acknowledges his earlier errors and offers a more conceptually sound explanation. From his observations, he is able to deduce how the micro-level events result in phenomena at the macro-level–the level at which most traditional chemical equilibrium questions are focused. Equally important was Andrew's willingness to question his understanding and the information provided by ChemLogo. While at first he indicated that there could never be more NO_2 in the reaction, he was willing to accept the possibility after disproving his hypothesis. His previous unquestioning attitude toward chemistry texts and instructors had left him with false confidence in his understanding. By focusing on the conceptual elements of the problem at hand, students in inquiry-based learning environments like ChemLogo can deduce more accurate and reasonable answers than they do with traditional curricula.

6.0 Concluding Remarks

This paper introduced a novel software package, ChemLogo, which aims to help improve student

understanding, retention, and application of the concept of chemical equilibrium. ChemLogo relies on modeling chemistry as emergent phenomena to provide an inquiry-based learning environment that enhances conceptual understanding. We observed several common misconceptions about chemical equilibrium in six advanced science undergraduates who we interviewed. Over the course of their interaction with ChemLogo, each student came to depend less on algorithms and rote facts and to depend more on conceptual approaches to problem solving and answer justification. Here we showed how one student, Andrew, successfully modified his definition and understanding of chemical equilibrium to answer questions with conceptual justifications based on his observations of the connections between micro-level and macro-level events displayed in ChemLogo. The practicality and benefits of each of these methods is a goal of future research. The work reported on herein is preliminary. We intend to study the impact of extended inquiry with ChemLogo in a ChemLogo- integrated secondary school curriculum. We'd like to look at issues of classroom integration, teacher learning and integration of model development in the chemisry classroom.

Inquiry-based learning environments such as ChemLogo show great promise for improving student understanding in chemistry as well as other physical sciences. The lack of concept-based reasoning and the use of rote memorization have resulted in students who lack the ability to solve problems that they themselves characterize as "basic." By presenting concepts on multiple levels together with multiple representations and providing students the opportunity for guided exploration with immediate feedback, learning environments such as ChemLogo can revitalize student interest and improve understanding.

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