How Computer Simulations Can Assist Model Generation In Students: Providing an Adaptable Structure to Guide Student Learning

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Abstract: Le Châtelier's principle and chemical equilibrium are considered two of the most difficult topics for students in high school chemistry, and despite the development of numerous simulations, software solutions have met with limited success. We present two case studies of expert teachers teaching Le Châtelier's Principle and show how the findings of the case studies have informed the design of a novel simulation. We have identified several key tactics used by these teachers that are not currently supported or enhanced by available simulations. Based on these studies, we have designed a novel simulation that 1) affords opportunities for model construction with analogies, 2) facilitates model evaluation by providing multiple reaction representations, and 3) guides learning by explicitly requesting predictions from students. This paper reveals strategies to promote model-based learning in chemistry and a design for an educational simulation that has been closely informed by model-based teaching practices.

Introduction

Although Le Châtelier described his principle of chemical equilibrium as "très simple" (O'Brien, 2002) it has been suggested that Le Châtelier's Principle is the most difficult concept for high school students to comprehend. Le Châtelier's Principle states that if a closed system at equilibrium is subjected to a change, processes will occur that tend to counteract that change (Hebden, 1998). Reasons provided for students' difficulties in understanding Le Châtelier's Principle include: the inherently abstract nature of the principle (Huddle and Pillay, 1996), and student conceptions that chemical equilibrium is an "equal state"(Gussarsky & Gorodetsky, 1990). Students are able to make observations of chemical processes at the macroscopic level, such as observing a colour change, but may not be able to state why these changes occur at a molecular level because they are not able to see the arrangement and motion of molecules, atoms or subatomic particles (Wu et al., 2001). Most traditional instruction in chemistry involves methods such as notes, exercises, labs and demonstrations that emphasize examining macromolecular phenomena. In order to meaningfully apply what is learned in secondary level chemistry, such as how gases diffuse and how chemical reactions occur, students need to understand chemistry at the molecular level. Individual molecular behaviour is unobservable, so students must make inferences about how molecules behave by observing chemical reactions. Researchers have also found that using computer simulations may afford opportunities to promote students' understanding of unobservable phenomena in science (de Jong, et. al., 1998; Stratford, 1997). However more recent studies have suggested that computer simulations can be more effective if coupled with guidance strategies (Kozma, 2000).

The GEM cycle is a teaching approach that aims to foster understanding of unobservable phenomena (Khan, 2002; Clement & Steinberg, 2002). This approach involves 1) *G*enerating an initial model, 2) *E*valuating the initial model based on new evidence and 3) *M*odifying the model if necessary (Khan, 2004, 2002). By repeatedly doing this, a highly robust mental model of the concept can be generated by the student.

The purpose of this study is to investigate how classroom activities and a simulation based on the GEM cycle can contribute to student understanding of two of the most challenging topics in chemistry: Le Châtelier's Principle and chemical equilibrium. This study is part of an ongoing, larger investigation of the different approaches used by students in their understanding of unobservable phenomena in science classrooms as they interact with computer simulations. In the following paper we discuss the findings from two case studies and make recommendations derived from our analysis in order to provide support for the design of our simulation.

We have designed a novel simulation that supports GEM cycle conceptual learning. This is achieved by using three features:

1) A prediction mechanism that explicitly asks students, using their current model, to predict the effects a system stressor will have on concentrations. This feature will afford opportunities to inspect aspects of students' prior models. Predictions will also help student evaluate their models and will provide an incentive to modify models that conflict with data.
2) An analogy feature that helps students explain how their initial model is representative of a larger chemical reaction. The analogy view is also integrated in the simulation to help explicate the connection between molecular and macromolecular phenomena. The analogy feature has been designed to support the generate model phase of the GEM cycle approach.
3) Synchronized multiple views or representations for a given chemical reaction help students develop temporally based conceptual links between different chemistry symbol systems. This feature is designed to provide students with more data to evaluate their models against and allow users to incorporate information based on their level of expertise, as suggested by Kozma (2000).

Related Work

Educators have directed considerable time and effort toward developing computer simulations to help students visualize concepts at the molecular level and connect chemistry in the classroom to what they can observe outside in their everyday lives (Steiff & Wilensky, 2003). Computer simulations are ideal tools for chemistry since students can interact with a system, change factors, variables, or rules and in some cases, receive feedback in the form of graphical outputs (Kozma, 2000; Stieff & Wilensky, 2003; Wu et al., 2001). Even though many current computer simulations in chemistry afford students with opportunities to visualize representations of molecules and manipulate them virtually, we are still searching for interactive tools that help students bridge the macromolecular with the molecular, encourage student self-reflection about unobservable phenomena in chemistry and scaffold model generation and evaluation. We believe our simulation provides these services.

Bridging the macromolecular with the molecular

According to Kozma (2000), understanding unobservable scientific phenomena requires indirect examination and an appropriate system of symbols to represent what is being observed. For example, chemical formulas are symbols that represent a chemical reaction. Furthermore, connecting symbolic and referent information in context is important for novices since they have difficulties linking symbols and the underlying scientific phenomena being investigated (Kozma, 2000). Along with Kozma (2000), Steiff & Wilensky (2003) suggest that teachers should use multiple representations to illustrate processes taking place at the microscopic level. Simulations such as 4M:Chem and Connected Chemistry provide tools and mechanisms for displaying multiple views of a chemical reaction, including concentration graphs, the chemical formula, macroscopic reaction views, and a molecular view of the chemical reaction (Kozma, 2000; Stieff & Wilensky, 2003). These multiple simultaneously viewed information streams provide students the opportunity to connect macromolecular reaction traits with molecular events. However, an environment's effectiveness is dependent on a student's cognitive strategies thus leading us to posit that greater scaffolding is needed to support students' understanding at the molecular level when simulations are being used (Kozma, 2000). Thus, we have designed a molecular view in the simulation interface and a series of classroom based activities that aim specifically to help students bridge their understanding of chemistry from a macromolecular science to one that involves molecules. Our simulation also provides scaffolding in the form of the prediction mode. We believe that more data will afford greater changes for student reflection if presented correctly, and we hope to examine this with our simulation.

Analogies

Staggers & Norcio (1993) state that mental model development is based on analogical or metaphorical reasoning. Learners generalize existing models to new phenomena through a process of mapping the old structural relations onto new relations (Gentner & Gentner, 1983). Therefore, in our simulation, we include an analogy view option in the interface. Prior research suggests that analogies can allow the learner to build on relationships already in prior knowledge rather than starting a model from scratch (Else, Clement, & Ramirez, 2003). Based on this, Clement and Steinberg (2002) argue that some of these relationships may be represented in concrete images or simulations to enhance visual perception of the phenomena. However, complex instructional analogies need to be presented with extensive direction from teachers in order to make them comprehendible (Glynn, 1991). Therefore, the curriculum we are developing includes model-based teaching activities designed to support student generation of analogies. Gussarsky and Gorodetsky (1990) found that students did not perceive an equilibrium mixture as a single entity but rather treated each side of the chemical equation independently as if it were a balance. The authors also noted that students interpreted equilibrium as a physical balance like riding a bicycle, or using a weighing balance/scale. In each of these interpretations, the equilibrium is incorrectly viewed as a static condition. Our simulation will use a weighing scale analogy to help students generate an initial model based on their intuition, but our analogy will clearly indicate that the chemical system is dynamic, even at equilibrium.

High School Case Studies

Case Study 1

A naturalistic case study was designed with the goal of examining how students construct understanding in chemistry and the kinds of teacher and student actions involved in this process. The objective was to analyse the GEM cycle in classrooms without computer simulations and to understand how an expert teacher helps students to understand unobservable and abstract phenomena in chemistry. Participants were students from two chemistry 12 classes in a suburban high school with an enrolment of 900 students. Class A had 23 students (16 males, 7 females), class B also had 23 students (10 males, 13 females), and both classes were studied during the Le Châtelier's Principle unit using qualitative analysis. Both classes were taught by a chemistry teacher with over 20 years teaching experience and a Master's degree in education. A classroom observation instrument was constructed (96.1% inter-rater reliability) to record the frequency of teacher and student actions that appear to foster model construction by time period. Classroom observation data consisted of field notes, digital camera recordings, and videotaping. These data were collected during lectures, labs, and small group activities on Le Châtelier's Principle. Pre and post student questionnaires were used to measure changes in student performance on Le Châtelier's Principle and one-on-one interviews were conducted with the chemistry teacher. Computers were not available to students, nor were any used during the duration of the unit. Labs were conducted within the same classroom.

Criteria related to each code in the observation instrument were designed according to the GEM cycle. The observation instrument was analyzed for the frequency of behaviours observed. Low and high frequencies of student and teacher behaviour during the Le Châtelier unit were used to inform the simulation's development.

Case Study 2

An evaluation study was carried out on an existing simulation referred to as the Davidson simulation (Blauch, 1998). Participants were students from two Chemistry 12 classes in a suburban school with a population of about 1400. There were a total of 40 students (25 females and 15 males). These students had not had any prior experience with computer simulations within the classroom. The study compared student understanding of Le Châtelier's principle from the two classes. Each class received the same instruction on chemical equilibrium and Le Châtelier's Principle through traditional methods (notes, examples, exercises, demonstration and labs) and used the Davidson simulation.

The only intentional difference between the two classes was that class A worked at the simulation in pairs whereas class B worked individually at each computer.

The Davidson simulation involves moving sliders to change the concentration, temperature, pressure or volume of the simulated system and seeing how the concentration or moles of the reactants and products change (Fig. 1). The simulation does not require students to predict the outcome before moving a slider and system changes are instantaneous. Students were evaluated on their understanding of Le Châtelier's principle using pre and post tests.

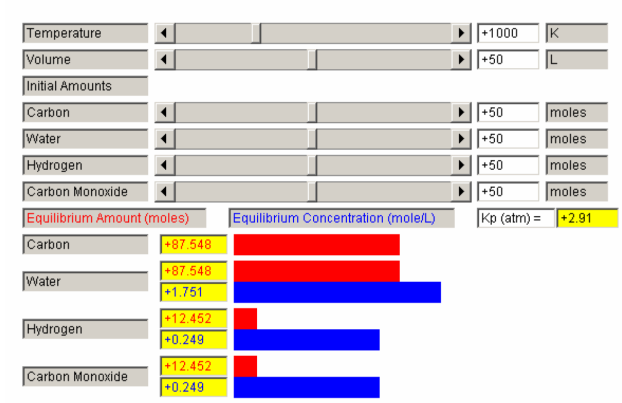

Figure 1: Screen capture of the Davidson applet used in case study 2.

Findings and Lessons Learned

Case Study 1

Frequency analysis of the classroom observation instrument indicated that the most regularly used Model Based Learning (MBL) characteristics applied by the teacher were (in order of frequency): quantitative problem solving, accessing prior knowledge, analogies, and explanations of conceptual models. These techniques were the only characteristics used at least once per lesson for at least three out of five lessons. Regular MBL characteristics used by students in more than three lessons were: quantitative problem solving (answering the teacher's question), explanations of conceptual models, comparisons, and evaluations. Learning techniques traditionally used with simulations such as isolating components, predictions, information gathering, and data analysis were not used more than once each by either the teacher or students during the five lessons. These findings suggest that problem solving, accessing prior knowledge, using analogies, evaluating models, and explaining conceptual models are important and presumably pedagogically effective in this classroom environment. Further, students may lack the exploratory techniques required to use previously designed simulations.

Approximately 30% of the class observation time involved a lecture with a whole class discussion, while 18.5% of observation time involved the teacher presenting a prepared lecture. Class participation was controlled to ensure that every student participated in discussions during a lesson. Hands on activities such as labs constituted 15% of the time, while individual writing, thinking, and reflecting occupied 11% of the observation time. The lack of hands on activity time suggests that the number of quantitative problem solving questions during lecture time may need to be reduced to find sufficient time to use a simulation. Furthermore, the emphasis on large group time may mean students are unaccustomed to working alone and motivating themselves. Any individual or small group oriented technology may need to provide additional motivation to students to be successful. Greater scaffolding and simulation structure may help students avoid "playing" with the simulation and help direct their discovery.

This case study's findings directly influenced our simulation design and we incorporated techniques that were frequently used by the teacher and students. Problem solving and model evaluation characteristics are addressed by our simulation's prediction feature and concentration graph, conceptual explanations are provided via a text dialog box, and our analogy feature involves analogies and accessing prior knowledge characteristics.

Case Study 2

Class A showed a significant ($p = 0.0256$) improvement in test scores, increasing from an average of 43.8% in the pre-test to 63.2% in the post-test. Class B's average changed from 51.3% in the pre-test to 58% in the post-test; a change that was not statistically significant. The only explicitly created difference in terms of instruction between the two classes was that class A collaborated in pairs and class B worked individually. This may be the reason why class A did significantly better than class B. The extra discussion that students were having during the simulation may have contributed towards a better understanding of the concepts. The students were motivated to think and apply themselves. Similarly, we expect that a more structured series of tasks will promote self reflection in novices.

The Davidson Simulation is one of several computer simulations on Le Châtelier's Principle we examined and may not be the best choice to illustrate the concept of chemical equilibrium. However, its use in Case Study 2 does make some points clearer for us regarding the design of a new simulation. Students are able to see the difference between changing concentrations and changing amounts (moles) of substances since both were displayed in text boxes for each chemical in the equilibrium. The Davidson simulation also shows how pressure and temperature changes affect the concentrations of reactants and products. Since the sliders and text windows only show the final effects of the stresses applied and do not show how the reaction re-establishes equilibrium, the Davidson simulation interface, in our view, may constrain potential understanding of Le Châtelier's Principle and its applications to chemical equilibrium. Students need to see how equilibrium is restored and this was not possible in the Davidson simulation.

The students also participated in a project where they brainstormed in groups to design a presentation showing how they see a chemical equilibrium and what changes take place before equilibrium is re-established. Students spontaneously used analogies such as different coloured crayons to represent reactants and products and the number of each crayon colour representing concentrations. Students did not receive specific instructions on what kind of presentation to make, nor were they asked to provide an analogy. The students spontaneously generated their own models, which they reviewed continuously with each other and the teacher at the teacher's request. It was observed that students were evaluating their models when they shared them with others and with their teacher. Findings from this study suggest that a successful simulation would be integrated into the peer and teacher-student relationship so that human interaction will influence model evaluation and modification. Further, this exercise suggests that students will be more critical and evaluative of their models if they discuss them with others. Finally, students seemed to have an affinity for using analogies to explain their models. These findings directly lead into our simulation's design and the corresponding curriculum we have developed to accompany it.

Our GEM Simulation

Based on the previous two research phases, we have designed a novel chemistry simulation that is geared toward supporting learning using the GEM cycle approach (Fig. 2). A team of computer scientists, educational researchers and teachers are using an iterative participatory design approach to help ensure ecological validity and to maintain a pedagogical focus during the simulation's development. This GEM simulation incorporates several features from previous chemical equilibrium simulations, such as a concentration graph, sliders, and a molecular view. Our simulation is novel, however, because it specifically addresses GEM cycle learning by addressing three key issues: reducing student difficulties in working with their initial mental model, facilitating model evaluation by providing a data rich environment, and providing structure to assist students in evaluating and modifying their models.

First, the GEM simulation simplifies initial mental model generation by providing an *analogy component*. The analogy view presents the chemical equilibrium simulation in terms of a weighing scale analogy, where familiar objects represent reactants on one side and products on the other (Fig. 2). This demonstrates how the reaction rates are balanced and how both reactants and products are still present. This is similar to the balance beam analogy used by Volland (1998) and should be intuitively understood (Gussarsky & Gorodetsky, 1990). The interaction between the scale and the scale's components are synchronized with the chemical reaction engine to ensure that the mapping between the analogy and the chemical concentrations is more explicitly coupled. The concentration graph then helps map analogical reasoning to empirical outputs since the scale shifting to the left always corresponds with an increase in reactant concentrations and/or a decrease in product concentrations. A scale shift to the right corresponds with concentrations changing in the opposite way. The scale analogy also demonstrates that forward and reverse reactions still occur at equilibrium, since chemicals continue to cross from one side of the scale to the other.

Second, student predictions are strongly encouraged with the *prediction feature*. If the prediction option is enabled, the computer manipulates chemical concentrations for students and they are instead asked questions via a text box about what the resultant concentration change will be (Fig. 2). This question is given as a 4-point multiple-choice question that must be answered before the simulation can be run. Thus students cannot randomly change concentrations but instead must follow a more structured behaviour. The prediction mode provides greater scaffolding to our simulation and is similar to the quantitative problem solving observed repeatedly during Case 1.

Finally, the *multiple view* simulation design provides a data rich environment for students to make an informed evaluation of their models. Our simulation has 5 different views of the simulation: a formula view, a slider view, graph view, analogy view, and molecular view. The formula view shows the chemical reaction formula and the chemical states involved while the slider view provides a control mechanism to students and supplies molarity data. The graph view plots concentrations for each chemical over time and can be used to "roll back" the simulation time so students can re-watch reaction events. Finally, the molecular view provides another chemical reaction analogy to students showing coloured spheres representing chemicals in the system. The spheres move, collide, and react with other spheres in the system and behave like a simplified molecular view of the reaction. Furthermore, the number of spheres of each colour always corresponds to the concentrations of each chemical. It is critically important that each of the five views is synchronized so a central simulation engine drove the display data to each view. The analogy and molecular views are not viewed at the same time due to screen real estate concerns.

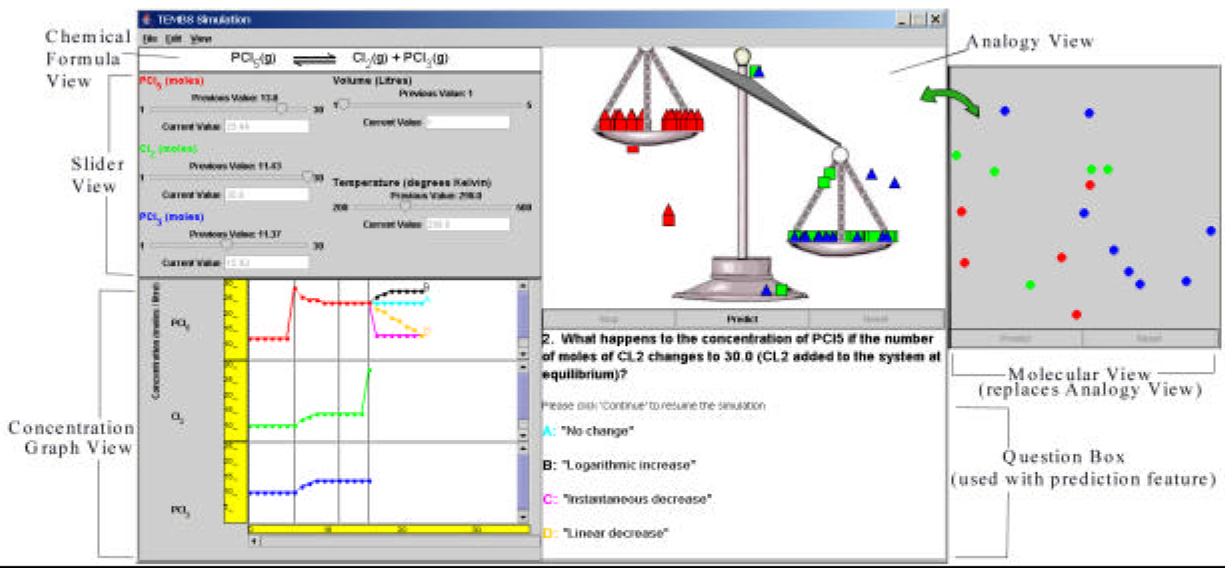

Figure 2: The GEM simulation interface demonstrating the histogram feature and prediction mechanism.

Benefits of the GEM Simulation

The GEM simulation provides features that uniquely enhance the GEM learning approach. However, to provide some customizability for teachers, we have made the analogy view and the prediction mode optional. They are activated or deactivated via the menu bar. Furthermore, these features can be turned on or off enabling students to adapt the simulation as their skills progress.

It has been observed, both in other equilibrium simulations and during Case 1 and Case 2 of this project, that students and teachers frequently use *analogies* when describing difficult topics. Analogous processes in science and in everyday life obey the same laws of nature and scientific rules. Unlike analogies used in other software, the GEM simulation will explicitly link the analogy's functionality to the chemical reaction. This stronger explicit connection between the reaction and the analogy, where the analogy view is mapped to scientific parameters, is beneficial for visualization and generation of mental models.

Previous research has demonstrated that multiple views of the same chemical reaction can be useful to students if implemented correctly (Kozma, 2000). We have used these finding, and our observations during Case 1 and Case 2 to guide our *multiple view* simulation design. The multiple synchronized views provide opportunities to not only evaluate how models succeed or fail at explaining the data, but also provide a mechanism for students to identify connections between multiple representations. Students can also replay reactions; something impossible to achieve in a chemistry lab. Furthermore, the rich environment supplies students with numerous ways to evaluate their models.

By making student *predictions* explicit, we hope to encourage users to think how their mental models match against real data and how they should be modified accordingly. Furthermore, the prediction mechanism provides a framework to encourage new students to think in a logical and sequential way. When students have answered a number of problems using the prediction mechanism, we hope that they will learn to evaluate reaction results in a similar way when they are manipulating concentrations in the open simulation. Although other software programs we have examined have required students to answer multiple-choice questions, we believe that our simulation uniquely allows students to transition between structured question and answer problems and an open simulation. We believe this progression is required for simulations to be truly effective for most students. We also believe that novice users would benefit from greater structure and this structure can guide them to modifying ineffective models.

Conclusions and Future Evaluations

Future evaluations of these three simulation components must be performed before we can examine the overall effectiveness of the GEM simulation. In May 2005 we will be introducing our simulation into four high school classrooms and running case studies examining the effects each simulation feature has on pedagogy, user opinion, and the time each student reflects on an answer. Future modifications to the simulation will focus on increasing student motivation to reflect on responses. Based on the outcomes of our studies and a literature review, we expect that peer performance, displayed as a histogram of class responses, will provide incentive for students to think before they answer questions. A *histogram view* will allow a student to anonymously compare his or her performance against the rest of the class. We wish to identify where this feature is beneficial and where it is detrimental. Examining how different analogies affect the GEM cycle is another possible research direction. Finally, we plan to improve incorporation of the simulation into the classroom by continuing to improve the classroom curriculum we are designing.

We attempted to design a simulation based on an established learning theory framework called GEM cycle model based learning. We proceeded to conduct two user studies to explore how model based learning is used in chemistry classrooms without a simulation, and then incorporated these features into our simulation's design. This resulted in a simulation that is both designed based on a theoretical foundation and also on practical teaching practices. We believe that by designing a simulation around the GEM cycle, enabling the simulation to be adapted to the skill set of the individual student, and by incorporating lessons learned though classroom observation, our simulation avoids many of the pitfalls associated with previous chemical equilibrium simulations.

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