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Pedagogic Roles of Animations and Simulations in Chemistry Courses

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Pedagogic Roles of Animations and Simulations in Chemistry Courses

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Foreword

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Before agreeing to publish a book, the proposed table of contents is reviewed for appropriate and comprehensive coverage and for interest to the audience. Some papers may be excluded to better focus the book; others may be added to provide comprehensiveness. When appropriate, overview or introductory chapters are added. Drafts of chapters are peer-reviewed prior to final acceptance or rejection, and manuscripts are prepared in camera-ready format.

As a rule, only original research papers and original review papers are included in the volumes. Verbatim reproductions of previous published papers are not accepted.

ACS Books Department

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Dedication

Jerry P. Suits (Editor) dedicates this book to J. J. Lagowski, who inspired and mentored him in this field.

Michael J. Sanger (Editor) dedicates this book to Thomas J. Greenbowe for mentoring him in chemical education research and the use of computer animations to teach chemistry concepts, and who still owes him much pizza.

Both editors would like to thank the Committee on Computers in Chemical Education of the ACS Division of Chemical Education (DivCHED).

Cover Image

Sugar and Salt Solutions. PhET Interactive Simulations, University of Colorado Boulder (see Chapter 5 for details).

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Chapter 1

Dynamic Visualizations in Chemistry Courses

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Chemistry can be a very difficult topic for students to understand, in part because it requires students to think abstractly about the behaviors and interactions of atoms, molecules, and ions. Visualizations in chemistry can help to make chemistry at the particulate level less abstract because students can actually "see" these particles, and dynamic visualizations can help students understand how these particles interact and change over time as a reaction occurs. This chapter provides a brief description of molecular-level animations, interactive chemistry simulations, and chemical systems and interactive simulations. In addition, this chapter includes a brief summary of the subsequent chapters in this book, which are divided into four different categories: Theoretical aspects of visualization design, design and evaluation of visualizations, visualizations studied by chemical education researchers, and visualizations designed for the chemistry classroom.

Introduction

Chemical educators have long recognized that students have difficulty learning chemistry concepts (*1–4*). Some of the reasons put forth to explain this difficulty include the ideas that: (a) Chemistry involves very abstract ideas that are not easily seen or understood (*1–4*), (b) Solving chemical problems often require students to access and process many different concepts and data at the same time (*4–6*), (c) In order to be successful at understanding chemistry concepts, students must be able to think and convert between the macroscopic,

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particulate (sometimes called the microscopic, molecular, or submicroscopic), and symbolic levels of representation (*3–5*, *7–9*), and (d) Students learning chemistry often have strongly-held preexisting conceptions that are inconsistent with scientifically-accepted theories and can interfere with subsequent learning (*3*, *10–14*).

Most visualizations (*15–17*) designed for chemistry instruction involve depictions of atoms, molecules, and/or ions and their interactions (the particulate representation), either as static images or as dynamic visuals including both animations (*18*) and simulations (*19*). The advantage of particulate visualizations (static or dynamic) in the chemistry classroom is that they provide students with a view of the behavior and interactions between the chemical particles, which are often abstract and difficult for students to generate on their own. Therefore, these visuals help make the abstract interaction of atoms, molecules, and ions more concrete (*3*, *16*, *18*), and can lower the cognitive load placed on the chemistry student (*4*, *5*, *19*, *20*). In addition, with proper instruction, these visuals can help students make connections between the macroscopic, particulate, and symbolic representations (*16*, *18*, *21*), which can lead to more scientific conceptions on the part of the chemistry student (*16–19*). Since many chemistry concepts require students to understand how the chemical systems change over time (e.g., reactants vs. products, before-and-after gas law experiments, equilibrium reactions, etc.), showing dynamic visuals can be especially helpful for students. Rieber (*22*) noted that dynamic computer animations were generally useful to students studying science, but can be distracting (and diminish learning) if the lesson does not involve visualization, motion, or trajectory. Both animations and simulations can be viewed as student-centered forms of instruction (*23*), which can support student learning as they develop a conceptual understanding of chemistry topics.

Some of the issues affecting students' abilities to learn chemistry concepts involve chemical theories [e.g., misconceptions related to the Kinetic Molecular Theory or Valence Bond Theory (*13*)] and chemical education theories [e.g., the interrelationships between macroscopic, particulate, and symbolic representations (*8*)]. However, some of these other issues are related to psychology or cognitive learning theories [e.g., Constructivism (*2*) or Cognitive Load Theory (*6*)] or theories on the optimal design and usage of multimedia programs (*24*, *25*). Therefore, the design and use of dynamic visualizations should take into account these and other chemical, chemical education, psychology/cognitive, and multimedia theories. In addition, dynamic visualization designers may want to focus on the issues of student learning objectives, students' prior knowledge, student interactivity and control, and assessments activities that will transcend mere recall while allowing students to develop their own mental models, to name but a few.

Molecular-Level Animations

According to Wikipedia (https://en.wikipedia.org/wiki/Animation), animation is "the rapid display of a sequence of static images and/or objects to create an illusion of movement." Computer animations depicting chemical processes at the molecular level have been studied for almost two decades

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(*20*, *26–29*), and have been shown to have promise in improving students' conceptual particulate-level understanding of chemistry (*18*). Most of these animations fall into one of two categories (*22*): *Presentation* animations (used to present new information or to elaborate on previously-presented information) or *conceptualization* animations (used to develop students' conceptual understanding without providing new information). Although molecular-level animations have been shown to improve student learning in chemistry, these animations can also lead to new student misconceptions that were not present before viewing these animations (*17*, *18*, *20*, *30*) and can prove distracting to students when the concepts that students are supposed to be learning are not visual in nature (*28*) or do not involve dynamic concepts such as visualization, motion, or trajectory (*22*). Because many of these molecular-level animations were designed to present new information to chemistry students, they often require only passive user inputs while simulations tend to emphasize a greater degree of student interactivity.

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Interactive Chemistry Simulations

A simulation uses a mathematical or logical model to recreate a situation or phenomenon. It allows the student to control the interactivity of the dynamic elements of the phenomenon being studied (*31*). When a simulation uses low levels of interactivity, students can control its instructional pace. This allows them to understand one part before going on to the next one. With high-level interactivity, the student can control the behavior of the simulation (*31*). Thus, students may input information (independent variables) to establish a system (e.g., an acid-base system) before they are exposed to the outcome (dependent variable). The outcome is thus a consequence of their decisions, which can be represented as a verbal or mathematical statement, a static visualization, or a dynamic visualization (animation). The goals of a simulation may include (a) to help students accurately estimate the likelihood of various outcomes; (b) to deliberately focus their attention on one part of reality at the expense of other parts; or (c) to see help students see how a system works by changing values for each variable, and then "running the simulation". The combination of these three goals allows students to make predictions about the behavior of the system and receive feedback about how the system works. When students are given the proper level of instructional support, they can use a properly designed simulation to discover scientific concepts (*31*). If there is a substantial amount of support provided to guide the student, then the simulation is focused on the guided discovery method. Conversely, when very little support is given, the simulation design allows the student to learn freely in the pure discovery method (*23*).

Chemical Systems and Interactive Simulations

Most of the chapters in this book refer to a *chemical system*, either explicitly or implicitly. An interactive simulation allows students an opportunity to explore chemical systems because they can manipulate various parameters in the system and then see the consequences of their decisions. One definition of a *chemical system* is "a group of interacting chemical species that exist in a

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dynamic relationship within a physical/chemical condition that responds in a predictable manner to changes in both internal and external conditions" (*32*). One pedagogic value of students modeling and simulating chemical systems is that their learning can progress from misconceptions (pre-conceptions developed from past experiences that are incompatible with the scientifically-accepted models and that are often very resistant to change) towards the scientific models that chemists have developed (*9*). The goal is to help students progress in the direction of becoming experts, who have developed the ability "to describe, explain, and predict the properties and behavior of matter (p. 188)" (*9*) as complex chemical systems. Thus, interactive simulations allow students to explore and begin to truly understand chemical systems.

Overview of the Chapters in This Book

Table I contains a summary of each chapter in this book including the authors' names, the types of theoretical frameworks used, the types of research methods used, a description of classroom applications, and the chemistry topics addressed in these chapters.

Theoretical Aspects of Visualization Design

Chapters 2-4 of this book focus on theoretical issues and concerns in developing and using animations and simulations to teach chemistry concepts. The theoretical frameworks described in these chapters not only include learning theories [such as Behaviorism (*33*), Cognitive Load Theory (*6*), and Vygotsky's Zone of Proximal Development (*34*)], but also describe design principles that are informed by educational research on learning with multimedia (*24*, *25*). Both of these frameworks can be used to improve the way dynamic visualizations are designed, created, and utilized in the chemistry classroom.

Stieff and Ryan (Chapter 2) used three theoretical frameworks based on cognitive learning theories to explore how molecular visualizations can link how students learn to the design of dynamic visualizations. This novel perspective on the theory-research-practice triad explores the ways that (a) short-term memory works by using both visual and auditory sensory information, (b) students acquire bits of knowledge that can be integrated to initiate their conceptual understanding of chemistry, and (c) visualizations can encourage students to interact with each other. Thus, molecular visualizations should be designed to focus on the 'heart of chemistry', which is the relationship between chemical structures and reactivity at the molecular level. When students explore this relationship, they are 'seeing' representations of unseen phenomena. While this chapter appeals mostly to simulation designers and chemical education researchers, it could also appeal to chemistry instructors who want to understand how the psychological mechanisms of understanding chemistry relate to visual representations of chemical processes.

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Table I. Summary of the Chapters in this Book.

Chapter	*Authors*	*Theoretical Frameworks*[a]	*Research Methods*	*Classroom Applications*	*Chemistry Topics*
2	Stieff & Ryan	CER, MM, PSY			
3	Schwartz, Milne, Homer, & Plass	CER, MM, PSY			Kinetic Molecular Theory
4	Gregorius	MM, PSY			Multiple
5	Lancaster, Moore, Parson, & Perkins	CER, MM, PSY	Qualitative		Multiple
6	Akaygun & Jones	CER, MM, PSY	Qualitative, Quantitative	√	Solubility, Equilibrium
7	Winkelmann			√	Laboratory Experiments
8	Keeney-Kennicutt & Merchant	PSY	Qualitative, Quantitative	√	VSEPR Theory
9	Kelly	PSY	Qualitative		Electrical Conductivity
10	Suits & Srisawasdi	CER, MM, PSY	Qualitative, Quantitative		Intermolecular Forces
11	Barak	CER, MM, PSY	Quantitative		Multiple
12	Williamson, Watkins, & Williamson	CER, PSY	Quantitative	√	Equilibrium
13	Rosenthal & Sanger	CER, MM, PSY	Qualitative, Quantitative		Oxidation-Reduction Reactions
14	Khan	MM	Qualitative, Quantitative		Equilibrium, Le Chatelier's Principle
15	Ashe & Yaron	CER, PSY		√	Kinetic, Thermodynamics
16	Fleming			√	Organic Reaction Mechanisms, Biochemistry
17	Martin & Mahaffy			√	Global Climate Change

[a] CER = Chemical Education Research, MM = Multimedia, PSY = Psychology.

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Schwartz, Milne, Homer, and Plass (Chapter 3) describe the results of a decade of work on the design, evaluation, and implementation of interactive multimedia simulations on kinetic-molecular theory aimed at high school students. The design of these simulations focused on presenting information that would not result in cognitive overload in the users (information design), where users had control of the simulations but with guidance to optimize their use (interaction or interactivity design), and using instructional supports like worked-out examples and instructional strategies to support reflection and student-student interactions (instructional tools and support). The authors also describe how these simulations were designed to help students develop mental models with strong connections between the macroscopic, particulate, and symbolic representations. The description of the decades of work done to create and evaluate these simulations should be very useful to simulation designers and chemical education researchers, as well as to chemistry instructors who use or may want to use simulations such as those described in this chapter.

Gregorius (Chapter 4) argues that the use of learning theories to guide the development and usage of animations in chemistry will lead to more effective animations and improved student learning. Gregorius describes how he used a variety of learning theories to develop and classroom-test chemistry animations with diverse populations of students enrolled in general chemistry courses over recent years. He found that instruction including the use of animations aligned to lesson objectives, peer discussion, and formal reporting procedures led to improved student grades. Gregorius describes examples of an animation designed based on behaviorist learning theory to assist students in learning the names of inorganic compounds and an animation designed based on cognitivist learning theory (schemata development and situated learning) to assist students in investigating the relationships between pressure, volume, amount of gas, and temperature under ideal gas conditions. This chapter should appeal to simulation designers, chemical education researchers, and anyone who is interested in understanding the interconnections between learning theories and effective chemistry animations.

Design and Evaluation of Visualizations

Chapters 5-8 of this book provide two examples of paired articles, in which the first chapter introduces and describes how the dynamic visuals were designed and created for use in chemistry instruction and the second chapter describes a chemical education research study performed to evaluate the effectiveness of using these dynamic visuals for chemistry instruction. Chapters 5 and 6 focus on interactive simulations created as part of the PhET Interactive Simulations Project. Chapters 7 and 8 focus on the virtual-world program *Second Life* and how it is being used to teach chemistry lessons.

Lancaster, Moore, Parson, and Perkins (Chapter 5) have developed and classroom-tested over 125 PhET interactive simulations in order to promote student conceptual understanding of science in general, and chemistry in particular. Their design was guided by three areas of research—cognitive research on how people learn, chemical education research on how students

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understand chemistry, and research on design features informed by educational technology and psychology. These simulations provide student interactivity and dynamic feedback to support students in the process of creating, controlling and understanding virtual chemical systems. The authors noted three issues related to the creation of simulations that were unique to the field of chemistry: Explaining macroscopic behavior in terms of particle interactions, representing physical processes in terms of symbolic and particulate representations, and using real-world examples to identify trends and develop models. This chapter could appeal to simulation designers, chemical education researchers, and chemistry instructors interested in using these (or similar) simulations in their classrooms who would like to see how simulations can be designed and used to help students explore and make sense of complex chemistry topics.

Akaygun and Jones (Chapter 6) used a PhET simulation on solubility equilibria to investigate how the degree of interactivity of an animation or simulation affected the mental models, attitudes, and perceived cognitive load of the dynamic visuals for high school and college students. They found that students used molecular features more often in their descriptions and mental models after they had experienced the visualization—regardless of its degree of interactivity. For the two groups of students, attitudes and perceptions of the cognitive load needed to use the animation or simulation were not significantly different. The researchers found that there was a negative correlation between perceived cognitive load of the visualization (whether or not the amount of information presented overwhelmed their ability to process it) and students' scores on the conceptual post-test on solubility equilibria. This chapter should be of interest to anyone interested in the relative effectiveness of animations with little student control versus simulations with more student control—designers, researchers, and chemistry instructors.

Winkelmann (Chapter 7) describes how virtual laboratory experiments are well suited for college chemistry courses and presents preliminary results of a study where chemistry students performed a virtual chemistry experiment within *Second Life*, SL (a popular virtual world program that allows virtual people and objects to interact). The students create a virtual representation of themselves (an avatar) that can move objects and interact with other avatars. Students can then perform a virtual experiment with the chemicals and equipment provided in SL. The experiment is analogous to a real experiment (i.e., acids and bases react with each other) but the danger of the chemistry laboratory is removed—although negative consequences should be established in the virtual world to correspond to real dangers. Winkelmann gave his students a pre-lab quiz and required them to analyze their virtual data and turn in a real lab report. While his students enjoyed the experience, they favored working with real chemicals. This chapter would be of interest to anyone interested in either supplementing the real laboratory or replacing it, provided that they understood the consequences of doing so.

Kenney-Kennicut and Merchant (Chapter 8) evaluated how performing several molecular creation and manipulation activities in the virtual world of *Second Life* affected students' understanding of the topic of VSEPR theory and the 3-D nature of molecules compared to students who worked with 2-D screen shots taken from SL. The two groups of students showed no significant differences

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in content knowledge, logical thinking skills, and visualization abilities after the experiment took place. Further analysis showed that the SL group exhibited an increased ability to interpret routine 2-D presentations of 3-D chemical structures, although many students in both groups could not interpret the 3-D information presented in 2-D drawings of molecules. Although they found potential benefits of SL, student attitudes of the SL group were split with regard to the potential benefits of SL use in chemistry courses. This chapter would be of special interest to anyone who is concerned with the potential benefits of synchronous (all students learning at the same time) or asynchronous (same lesson but performed different times) activities, such as use of simulations, videos, games, quizzes and interactions with virtual chemical species.

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Visualizations Studied by Chemical Education Researchers

Chapters 9-14 of this book describe the results of chemical education research studies on the use of animations and simulations. The research presented in Chapters 9 and 10 focused on evaluating the instructional effectiveness of simulations—Chapter 9 looked at instructor perceptions as a way to design instructional scaffolds with the ultimate goal of improving student learning from simulations, while Chapter 10 evaluated how the use of a simulation affects students' content knowledge and mental models. The research presented in Chapters 11-13 compared how different instructional conditions affected students' chemistry content knowledge and other cognitive skills. Chapter 11 looked at the effect of using 3-D visualizations and active learning strategies (compared to 2-D static pictures and passive learning techniques) on students' content knowledge and their ability to think and create arguments at the particulate level. Chapter 12 compared the content knowledge and mental rotation ability of students creating particulate pictures using a 3-D animation program or a series of 2-D note cards. Chapter 13 compared the particulate-level explanations of students viewing a more simplified animation followed by a more complex animation of the same chemical reaction to the explanations of students viewing these two animation in the opposite order. Chapter 14 consisted of two research studies; one comparing how a single group of students interacted with a simulation including a dynamic analogy-based depiction, and one comparing how a group of students viewing the dynamic analogy performed compared to a group of students in which the dynamic analogy was disabled.

Kelly (Chapter 9) studied how chemistry instructors conceptualize chemical phenomena at the atomic/molecular level. Her rationale for conducting this study was that instructors serve as the interface between visualization designers (by selecting and using particular products) and their students (by providing a classroom context where visualizations of phenomena can be linked to understanding). She found a great variety in the 'mental models' of the instructors, which spanned from using key features to show simplistic representations to those exhibiting more updated and complex scientific conceptions of the molecular phenomena. The former allows students to bridge from one level of understand to another, while the latter is more likely to ensure accuracy. These findings may relate to how much instructional support (scaffolding) students need to understand

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visualizations. This chapter could appeal to everyone—including chemistry instructors who can see that their advise is being solicited and used, researchers who study the effectiveness of instruction using visualizations, and simulation designers whose work can be improved through the use of this vital information.

Suits and Srisawasdi (Chapter 10) studied how the use of an interactive simulation they created affected students' content knowledge and mental models related to hydrogen bonding in water. The simulation used instructional scaffolds to help students relate the macroscopic property of contact angle in water to the particulate property of hydrogen bonding forces. They found that (prior to instruction) low-, medium-, and high-achieving students had different content knowledge (low < medium < high), different particulate-level mental models (low ≈ medium < high), and similar macroscopic-level mental models (low ≈ medium ≈ high). After using the interactive simulation, each set of students showed significantly improved content knowledge and particulate- and macroscopic-level mental models, but the initial differences in these three groups did not change. For the particulate-level mental models, each group showed fewer misconceptions and more correct conceptions after using the simulation. This chapter should be of interest to simulation designers and chemical education researchers as an example of how to evaluate the effectiveness of a chemistry simulation, and to chemistry instructors thinking about using simulations in their classrooms.

Barak (Chapter 11) performed three experiments using students at different educational levels to study the effect of actively interacting with 3-D dynamic visualizations compared to passively viewing 2-D static drawings. The first study used animated movies to explain scientific concepts to elementary students, the second study used 3-D molecular visualizations to teach high school students about the structure-function relationship of biomolecules, and the third study asked college students to use 3-D molecular visualizations to help in writing weekly reports about the structure and usage of chemicals. This study showed that students actively using the 3-D visualizations showed greater conceptual understanding; greater ability to convert between 2-D, 3-D, and textual representations; greater ability to convert between macroscopic, particulate, symbolic, and process representations; and stronger molecular explanations and arguments with respect to their peers using the 2-D static pictures. This study could appeal to simulation designers and educational researchers, but should be of special interest to elementary and high school teachers as a model of effective ways to incorporate a combination of dynamic visualizations and active learning strategies in their classroom.

Williamson, Watkins, and Williamson (Chapter 12) compared the chemistry content knowledge, mental rotation ability, and attitudes of students who were asked to model physical and chemical equilibrium reactions using either an animation program (ChemSense) or a series of note cards. They found that both groups of students showed improvement in their content knowledge of physical and chemical equilibria and their mental rotation ability; however, these scores were not significantly different when the two groups of students were compared. One possible explanation for this lack of difference was that many students using the note cards tended to create a step-by-step series of pictures that largely resembled an animation. This study also found that male students showed better mental rotation abilities than female students, and males showed a larger increase in their mental rotation abilities after the study compared to females. Although this study should be of interest to animation designers and chemical education researchers, it should be especially interesting to chemistry instructors since it shows that students who create visuals using an animation program or note cards can improve their chemistry content knowledge and spatial thinking skills.

Rosenthal and Sanger (Chapter 13) investigated whether the sequence of viewing two animations on the same chemistry topic (oxidation-reduction reactions) should proceed from simplified to complex or vice versa. Learning theories and common sense could argue for either of these sequences because both are representations of molecular phenomena. The authors found that the complex-to-simple sequence of animations led to improved student understanding of this complex chemical topic. This sequence appeared to use the more complex animation to grab students' attention, then showing the simpler one helped students explain the chemical reaction. When students viewed both animations, they had difficulty relating the concepts depicted in one animation to the other because the same chemical species (copper/silver atoms, copper/silver ions, etc.) were often depicted in different ways. The role of water in this reaction was somewhat confusing to students—was it just a spectator, an active participant in the chemical reaction, or the driving force of the reaction? This chapter should be of interest to anyone who wonders about the instructional effectiveness of animations—designers, researchers, and chemistry instructors.

Khan (Chapter 14) performed two studies to determine how a multifaceted simulation of an equilibrium system using a two-pan balance as a dynamic analogy of the equilibrium process can improve student understanding of chemical phenomena. In one study, she evaluated students' understanding of equilibrium concepts after they had viewed the analogy-based simulation. After viewing the simulation, students showed a partial improvement of the understanding of the behavior of molecules before and right after a chemical is added to disturb equilibrium, but still had difficulty describing the distribution and composition of the particles after equilibrium was reestablished. The other study compared students' conceptual understanding of Le Chatelier's principle after using the simulation either with the dynamic analogy enabled or disabled. Khan found that students viewing the simulation with the dynamic analogy enabled had a better understanding of Le Chatelier's principle than those viewing the simulation without the dynamic analogy. This chapter may especially appeal to chemistry instructors who are interested in how to teach chemical systems because it gives an elaborate example of visualizations that were studied and used in chemistry classrooms.

Visualizations Designed for the Chemistry Classroom

Chapters 15-17 describe how specific dynamic visualization programs and modules were designed and how they should be utilized in the chemistry classroom to improve student learning. Chapter 15 describes the steps used to create analogy-based animations for the chemistry classroom and describes a couple of examples related to kinetics and thermodynamics. Chapter 16 describes visualizations based on modeling organic reaction mechanisms and viewing 3-D models of biomolecules. Chapter 17 describes the process of creating and the optimal use of several simulation modules focusing on the chemistry concepts related to global climate change.

Ashe and Yaron (Chapter 15) argue that appropriately designed simulations incorporating analogies involving everyday objects can help students learn abstract concepts needed to organize their content knowledge. They describe the steps used to create these analogies in which the simpler or more familiar situation (base) is mapped onto the more complex or abstract concept (target). An example discussed in this chapter is the use of cardboard box (and its relative stability with respect to its center of gravity) to serve as an analogy for the reaction-coordinate diagram used for chemical reactions. They also describe another analogy to explain the relative populations (based on the energies) of the reactant, activated complex, and product states using a container filled with balls containing tiers of different heights placed on a vibrating platform. This chapter should be extremely valuable to chemistry teachers who are looking for new and interesting ways of teaching chemistry concepts to their students using simple analogies as a way to improve conceptual understanding.

Fleming (Chapter 16) provides an historical description and analysis of the advantages and disadvantages of several visualization programs created to teach two topics that students often have difficulty learning—organic reaction mechanisms and visualization of 3-D biomolecules. Included in this summary is a description of a multi-representational animation of an S_N2 reaction that synchronizes changes in structure from the reactant to the transition state to the product with the progress-of-reaction graph (reaction-coordinate diagram). This animation allows the student to stop it, study it, and to carefully watch this inversion mechanism as a way to truly understand it. The 3-D biomolecular animations described in the chapter provide biochemistry students with a 3-D perspective that allows students to rotate these molecules in order to understand their structure-function relationships. This chapter would be especially valuable to organic chemistry instructors who recognize that students need help in visualizing organic reaction mechanisms, and biochemistry instructors who would like their students to 'explore' complex the 3-D structures of biomolecules.

Martin and Mahaffy (Chapter 17) describe the rationale used to create a set of simulations within the rich context of the complex chemical systems present in global climate change, and describe in detail how these modules can be used in the chemistry classroom. The interactivity and feedback of these simulations allowed the authors to monitor and assess student misconceptions related to this complex, real-world system. These interactive simulations were embedded in chemistry course content to foster student engagement in more interactive ways (e.g., probing evidence and constructing mental models built upon fundamental science concepts). The authors point out that scientists who study the science of global climate change use simulations that are based on real-world data from atmospheric studies. Thus, students are learning from pedagogic simulations using the same real-world data that scientists use to construct scientific models of climate changes. This chapter should be of interest to chemistry instructors who recognize the value of real-world chemistry applications, simulation designers who seek examples of embedding simulations in a complex chemistry topic, and chemical education researchers who want to study simulations within a complete instructional context.

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Chapter 2

Explanatory Models for the Research & Development of Chemistry Visualizations

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In this chapter we present the utility of three theoretical frameworks used by the cognitive and learning sciences communities to inform the research and development of computer visualizations for teaching chemistry. First, we review Baddeley's (1974) tripartite theory of memory to motivate studies on the design of new representational systems in molecular visualizations. Second, we review diSessa's (1988) knowledge-in-pieces theory to motivate studies on the potential of new visualizations to promote conceptual change. Third, we review Bandura's (1977) social cognitive learning theory to motivate studies regarding the role of new visualizations in promoting social interactions. We present each model by reviewing its historical development in the context of research on learning and fundamental components, and the specific implications of the model for research on chemistry visualizations. We argue that each theory offers a unique explanatory mechanism for the potential of visualizations in the classroom and expands the scope of new research programs beyond studies of efficacy and effectiveness.

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Introduction

Visualizations are increasingly prevalent in secondary and post-secondary chemistry classrooms where they afford students greater access to the central concern of chemistry, namely structure and reactivity (*1*). The advancement of new educational technologies presents unprecedented opportunities for educators to provide students with access to visual representations of atomic structures, molecular interactions, and large datasets to support chemistry learning. Today, students and teachers at all levels of instruction employ a wide array of visualizations that allow them to conduct "molecular experiments" that demonstrate physical and chemical processes. The benefit of such tools for improving the learning of chemistry appears self-evident: because these tools provide visual representations of the unseen phenomena of study, students who use them will develop a richer and more accurate understanding of chemistry concepts.

Visualizations have seen increasing use in the classroom; however, evidence of their effectiveness for improving learning and understanding has been unreliable (*2*). Relatively few studies have demonstrated that these new technologies produce reliable gains in student engagement, achievement, retention, or affect. In some cases, students who learn from visualizations achieve higher scores on summative assessments than students who do not use visualizations (*3*, *4*); elsewhere, visualizations produce no gains (or even decrements) in achievement (*5*, *6*). The discrepancy of these findings raises important questions about the underlying mechanisms that explain the efficacy of visualizations for teaching chemistry specifically. In this chapter, we argue that unreliable reports on the efficacy of visualizations, specifically animations and simulations, are artifacts of studies that include unprincipled implementations of visualizations in learning environments that do not instantiate rigorously tested design principles.

Current approaches to the design and study of visualizations in chemistry make use of two major theoretical frameworks developed within the chemistry education research (CER) community. Although these frameworks are often conflated, they are different in kind. First, chemistry education researchers have long argued that students face significant challenges coordinating the submicroscopic, macroscopic, and symbolic descriptive "levels" in the domain (*7–9*). Citing such challenges as the central obstacle for learning in the discipline, many designers have constructed new visualizations that present multiple levels simultaneously (*10*). According to this framework, visualizations are effective because they relieve the student from the burden of identifying the relationship between multiple levels. Second, chemistry education researchers argue that chemistry is difficult to learn because students must coordinate the meaning of multiple representations (*11*, *12*). Multiple symbolic representations, such as empirical formulas and structural diagrams, are used to refer to the same submicroscopic entities, and students do not clearly perceive the relationship among all available representations. To address this issue, designers have built new simulations that present multiple, linked representations simultaneously (*13*,

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14). According to this framework, the efficacy of visualizations results from interfaces that help students relate representations.

Although the application of these two frameworks has yielded important insights into the design of chemistry visualizations, they are both limited in their power to explain how and why visualizations can promote chemistry learning across the curriculum more broadly. A more comprehensive account of the role of visualizations is needed to realize their full potential in the chemistry classroom. Here, we aim to stimulate discussion about the role of visualizations and the design of research programs that investigate their efficacy. To that end we examine three models, which are widely employed by the communities of cognitive and learning scientists, that can account for the underlying mechanisms of learning with visualizations in general and provide specific predictions about the design of learning environments that make use of chemistry visualizations. Importantly, these models are based on empirical data of student learning and motivate design principles that give systematic structure to visualization interfaces and learning activities. As such, each leads to strong recommendations about when and why visualizations are effective in various contexts.

What Is a Chemistry "Visualization?"

Visualizations in chemistry take many forms, and the word "visualization" has been used in multiple ways throughout the chemistry education research literature *(cf.* (*1*, *14–18*)*)*. For the sake of this chapter, we are restricting our use of the term visualization to *any virtual environment that represents dynamic interactions of submicroscopic (or subatomic) phenomena*. We have restricted our definition in this way because prior research indicates that a primary challenge learning chemistry involves mechanistic reasoning in chemistry (*19*). That is, students' struggle to understand how particle behavior (*20*) and, to a lesser extent, structure (*21*) are related to the chemical and physical properties of substances. As such, technologies that include visual representations of particle structure, motion, and interaction hold the most promise for helping students to develop a coherent understanding of particle behavior. We acknowledge that many chemistry visualizations may include representations of other descriptive levels of phenomena, such as macroscopic pictures or symbolic representations (*22*); however, we believe these technologies do not facilitate mechanistic reasoning like submicroscopic visualizations.

A significant consequence of our definition is that we exclude visualizations that demonstrate simulations of macroscopic experimental techniques (*23*) or facilitate the memorization of different symbols in the chemistry classroom (*24*). This definition also excludes submicroscopic simulations that allow manipulation of chemical structures without showing dynamism, such as electrostatic potential maps (*25*) or Jmol (*26*). Our intent is not to diminish the relevance of these types

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of visualizations for learning chemistry. To the contrary, we believe that these types of environments can be effective in a variety of contexts, but the underlying models that motivate their use are different from those models that we discuss in this paper.

Excluding visualizations of these kinds, we note that our definition captures several learning environments widely employed in secondary and undergraduate classrooms that have been produced by the CER community (Figure 1), such as *PhET* simulations (*10*), *VisChem* (*27*), *Molecular Workbench* (*28*), *Electronic Learning Tools* (*29*), and *The Connected Chemistry* (*30*). Notably, these learning environments offer visualizations of different kinds, such as animations and simulations. *Animations* include those visualizations that display a scripted sequence of events for passive viewing. These visualizations often permit students to set an initial set of conditions and limit the displayed information to highlight only those features most relevant to the represented concept. Animations can be effective tools to direct students to focus their attention on a specific aspect of a phenomenon at the submicroscopic level, such as the process of dissolution (*27*). In contrast, *simulations* use empirical data and algorithms to display dynamic interactions resultant from particle motion in real time (*31*, *32*). Today, many simulations allow students to exercise greater agency than animations by including interfaces that allow manipulation of system variables and control of a microworld where they can construct virtual experiments to test predictions in a virtual environment that has a high degree of fidelity to the physical world (*33*).

Designers embed animations and simulations in learning environments that can differ on five dimensions: *control*, *interactivity*, *feedback type*, *feedback amount*, and *representational consistency* (*33*, *34*). *Control* refers the extent to which a student can set initial system parameters and explore the visualization in ways of their own choosing. *Interactivity* refers to the extent to which a designer provides the student with opportunities to influence the behavior of the system in real time. For example, two simulations from *The Connected Chemistry Curriculum*, *Real vs. Ideal Gas* and *Chemical Changes*, differ in both interactivity and control. Both simulations were designed in a microworld that uses a physics engine that updates the position and velocity of each particle dynamically and probability models determine the outcome of particle collisions in real time. In the *Real vs. Ideal Gas* simulation (Figure 2), students have little control over the microworld: the only variable that the designers allow the students to manipulate determines whether the simulation models ammonia as a real gas or an ideal gas. Similarly, students can interact with the simulation in only one way. As the simulation runs, they can toggle between real and ideal gas behavior.

In contrast, the *Chemical Changes* simulation (Figure 3) is highly interactive as it includes multiple variables (e.g., volume, heat, and mass) that students can manipulate in real time. As students modify system parameters, the simulation updates and displays changes to dependent variables. Because students are able to select many possible starting conditions and modify how the simulation runs as they wish, students are able to exercise more control over their learning by running many different simulations that have unique parameters. Visualizations of this kind give students more agency over their learning of chemistry.

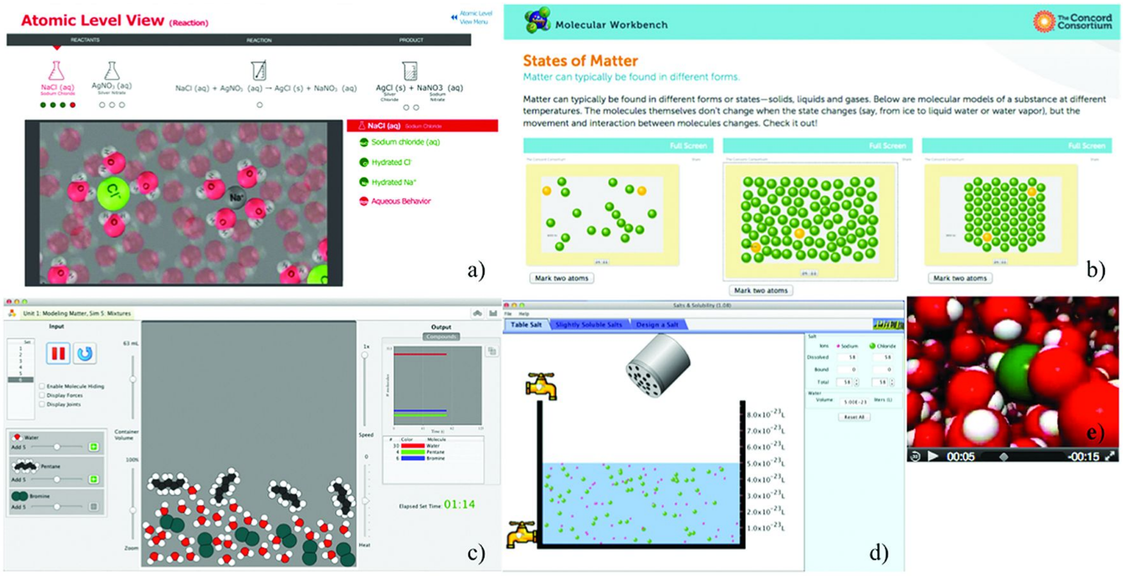

Figure 1. Examples of extant animations and simulations produced by the chemistry education research community. Screenshots of a) Electronic Learning Tools Atomic Level View animation (Courtesy of Electronic Learning Tools (www.chemteam.net)), b) Molecular Workbench States of Matter simulation (Courtesy of The Concord Consortium (http://concord.org). Molecular Workbench simulations can be found at http://mw.concord.org.), c) The Connected Chemistry Curriculum Mixtures simulation (Courtesy of The Connected Chemistry Curriculum (www.connchem.org)), d) PhET Salts & Solubility simulation (Courtesy of PhET Interactive Simulations at the University of Colorado. PhET simulations can be found at http://phet.colorado.edu) and e) VisChem Chemical Reactions Complexation animation (Courtesy of VisChem). (see color insert)

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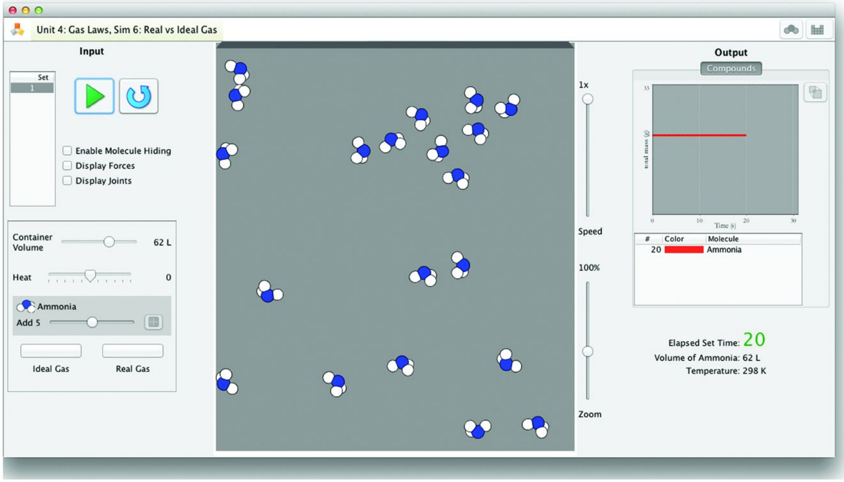

Figure 2. A screenshot from The Connected Chemistry Curriculum Real vs. Ideal Gas simulation that offers a low level of interactivity and offers students limited control of the variables. Courtesy of The Connected Chemistry Curriculum (www.connchem.org).

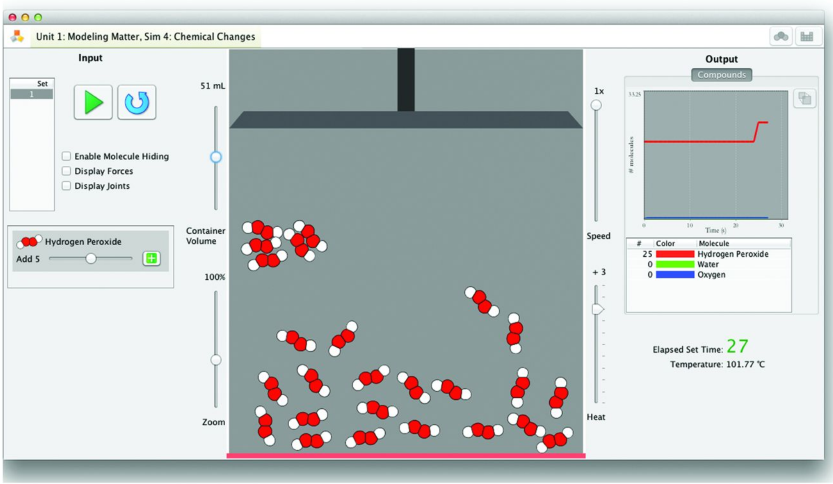

Figure 3. A screenshot from The Connected Chemistry Curriculum Chemical Changes simulation that is highly interactive and offers students control of several variables. Courtesy of The Connected Chemistry Curriculum (www.connchem.org).

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Feedback type refers to the quality of feedback users receive about the appropriateness of their interactions and the results of their choices when working in a microworld. This feedback can be explicit when the interface offers clear and direct evaluative information to the student; alternatively, feedback can be implicit when the interface only indirectly provides such information. *Feedback amount* refers to how often a user is presented with feedback. Visualizations can provide users with limited or extended feedback. Taken together, the type and amount of feedback can range from limited and implicit to extended and explicit. For example, the *PhET Build a Molecule* simulation offers limited and implicit feedback by prohibiting students from building incorrect structures. When a student tries to create an energetically unfavorable bond between two atoms, the simulation responds by forcing the two atoms apart. No explicit feedback is provided that explains why the bond does not form, why two atoms were forced apart, or guidance to a correct solution.

Alternatively, the *Electronic Learning Tools Atomic Level View* animation offers students extended, explicit feedback while interacting with the interface. As shown in Figure 4a, students are presented with responses they produced prior to working with the animation and asked to reflect upon those responses after viewing an animation. The students are then prompted to construct a new image to represent how their understanding has changed. When a student constructs an incorrect diagram (e.g. incorrect ratio of ions, lack of water), the interface prompts the students with questions to help the students construct an accurate diagram. For example, in Figure 4b, the ratio of sodium ions to chloride ions is incorrect and the question "What is the ratio between the sodium and chloride in the solution?" appears. Importantly, some learning environments do not provide feedback in the visualization itself and instead rely on teachers or other curricular materials to provide feedback.

Lastly, *representational consistency* refers to the extent to which a microworld makes systematic use of a system of representations that link the visual images displayed to the objects and phenomena they represent. *Electronic Learning Tools, ChemVis* and *The Connected Chemistry Curriculum* all demonstrate a high degree of representational consistency by assigning a specific size and color to each element on the periodic table. For example, water molecules in both learning environments are represented with two white balls (hydrogen atoms) and one red ball (oxygen atom). Thus, a student can anticipate that any red ball in any visualization refers to an oxygen atom. In contrast, *PhET* simulations and *Molecular Workbench* visualizations demonstrate a low degree of representational consistency. For example, in *Molecular Workbench* water is represented as two white circles (hydrogen atoms) attached to another red circle (oxygen atom) in the *Solubility: Dissolving Salt in Water* animation (Figure 5a), but as a generic two atom polar molecule in the *Intermolecular Attractions and Solubility* animation (Figure 5b).

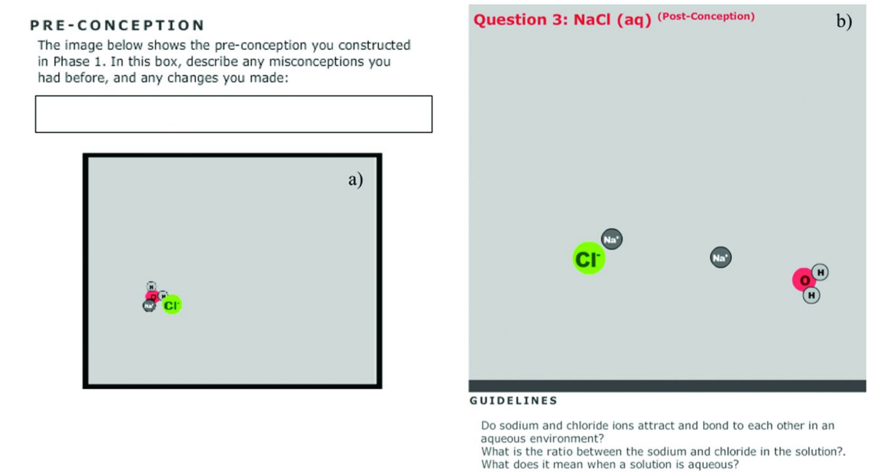

Figure 4. Screenshot of the Electronic Learning Tools animation feedback system. a) Students are prompted to reflect on their preconception after watching an animation b) Students are given explicit feedback in the form of prompting questions when incorrect configurations have been selected. Courtesy of Electronic Learning Tools (www.chemteam.net).

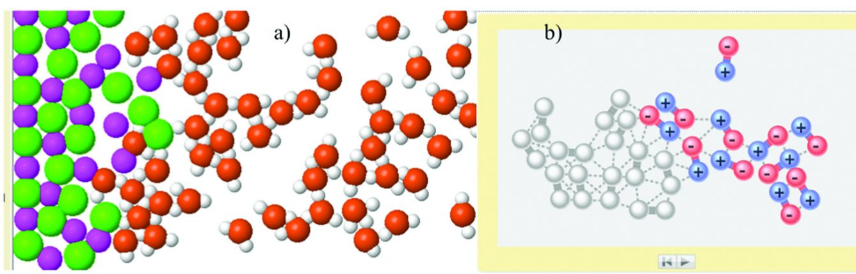

Figure 5. Examples of representational inconsistency in Molecular Workbench visualizations. Elements and molecules are represented different between simulations. Courtesy of The Concord Consortium (http://concord.org). Molecular Workbench simulations can be found at http://mw.concord.org.

Three Explanatory Models for the Efficacy Chemistry Visualizations

With a working definition of a "chemistry visualization" and a list of features common to several learning environments that employ them, we next review three models of human learning that we believe can inform design and research on the efficacy of visualizations. First, we examine the potential of visualizations to support retention of domain concepts according to the tripartite model of working memory (*35*, *36*). Second, we explore the potential of visualizations for promoting conceptual understanding when embedded in lessons using the contemporary "knowledge-in-pieces" model of conceptual change (*37*, *38*). Finally, we review the potential of visualizations for supporting social interactions in chemistry using one model of social cognitive learning (*39*, *40*).

We believe these models permit the CER community to extend their work on visualizations beyond simple assumptions that visualizations are effective because they help students "see" molecules and atoms that are otherwise invisible to the naked eye. Each model supports a discrete set of research questions that warrant investigation in the context of chemistry instruction; together, the models offer a convergent set of design principles for building new visualizations. Of course, it is beyond the scope of this chapter to review each model in extensive detail. Rather, it is our hope that an overview of these theories will spur the chemistry education research community to seek ways to apply these models in their work to produce more innovative designs and more rigorous empirical studies that establish the effectiveness of visualizations.

The Tripartite Model of Working Memory

The first model we review is Baddeley & Hitch's tripartite model of working memory (*35*, *36*, *41*). The tripartite model of working memory is one of several information processing models proposed by cognitive scientists to explain human memory. *Information processing models* are cognitive models that attempt to describe the organization and structure of memory and the processes by which information is transferred and transformed within and between these structures. The first of these models was put forward in the late 1950s in an attempt to explain complex learning and information recall, and several models have been proposed, revised, and abandoned over the past 60 years (*42*, *43*). Importantly, the central concern of these theories is to explain how humans acquire, retain, and recall information that is experienced in the world (as opposed to generated in the mind).

The rise of information processing models in the 1950s was coincident with the rise of computing technologies at the time. The success of hardware that partitioned information among hardware components that stored information for long-term retention in one component (i.e., the hard drive) and components that retrieved and manipulated that information to execute programs (i.e., RAM), fueled theoretical models that included similar partitioned components in the human mind. There is much debate about whether cognitive science's information processing models of mind or computer science's hardware architectures were developed first; however, the cognitive science community is agreed that regardless of which field predates the other, the two grew in tandem (*42*). Advancements in one area led to insights in the other as engineers and psychologists collaborated to design hardware components that better simulated human problem solving and provided a test bed for experiments aimed at furthering our understanding of human memory.

Among the various models still employed by cognitive scientists and learning scientists today are the "modal model" (*44*), the "levels of processing" model

(*45*), and the "tripartite model of working memory" (*35*). Researchers in various disciplines employ each of these models to explain how students remember disciplinary concepts and apply those concepts for problem solving. Although each theory maintains unique descriptive models of human memory, all share a common commitment to an underlying structure that involves the storage and activation of mental representations of information. Although Atkinson and Shriffin's model did not rigidly define the structure of memory, the later models posited that human memory is divided into multiple components that include the *sensory register*, *working memory*, and *long-term memory*. Briefly, the sensory register is responsible for filtering information in the world and translating that information into mental representations that can be manipulated and stored for later recall. Working memory is responsible for manipulating mental representations for problem solving and executing processes that transfer these representations into and out of long-term memory. Finally, long-term memory is responsible for the storage of mental representations for retrieval and later use.

There are important differences among the information processing models with regard to the cognitive architecture and the information handling processes responsible for the selection, storage, and retrieval of information. Cognitive scientists do not consider the models equivalent, and each model leads to different predictions about learning and human behavior. Increasingly, research in neuroscience supports component models with evidence that specific neural structures are responsible for storage and processing at different stages of learning. Between the component models, we believe that Baddeley and Hitch's tripartite model of working memory provides the most fruitful explanations of the effectiveness of animations and simulations and offers a sound theoretical framework to support further research on the efficacy of new visualizations in chemistry. Indeed, Baddeley and Hitch's model (*35*, *46*) is the foundation for several contemporary learning theories, such as Mayer's (*47*) Theory of Multimedia Learning or Sweller's (*48*) Cognitive Load Theory, which have been used to explain the efficacy of educational technologies more broadly.

Although these later two theories have found much traction in the chemistry education research community, we believe that the community might benefit from a "return to first principles." These contemporary theories offer clear explicit principles (e.g., design interfaces that do not require students to read text simultaneously while viewing an animation (*47*)); however, the underlying mechanisms by which visualizations can improve retention and recall is best explained by the original tripartite model of working memory. Similarly, we believe that research that makes use of the tripartite model of working memory can produce more precise recommendations about which concepts are suited for learning via animations and simulations. It is our hope that a review of the model can motivate new discussions among chemistry educators about how best to design new interfaces and to analyze the relative affordances of those designs.

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Features of the Tripartite Model of Working Memory

The tripartite model of working memory focuses narrowly on the structure and processes of Atkinson and Shiffrin's short-term memory. As indicated in Figure 6, Baddeley and Hitch proposed that working memory itself is partitioned into three components: the *auditory loop*, the *visuo-spatial sketchpad (VSSP)* and the *central executive*, each with unique functions. The first two components are responsible for maintaining and transforming information received from sense organs and the central executive is responsible for coordinating the function of working memory. As an "aural buffer," the auditory loop maintains and manipulates auditory information sensed via the ears as sound images. The visuo-spatial sketchpad maintains and manipulates both visual and spatial information. At the time, Baddeley and Hitch emphasized that the VSSP received information primarily from the eyes, but today the model has expanded to include information received from both kinesthetic and proprioperceptor organs (*35*, *49*). Importantly, the VSSP is believed to maintain representations that are both visual (e.g., "pictures in the mind") as well as spatial (e.g., judgments of relative distance). Finally, the central executive is responsible for regulating the processes of the VSSP and auditory loop as well as coordinating information to and from the long-term memory.

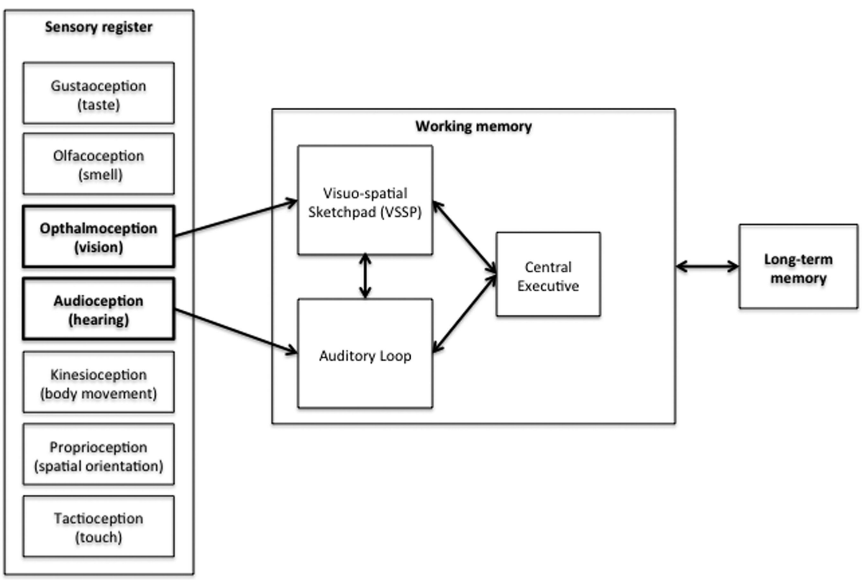

Figure 6. Conceptualization of Baddeley and Hitch's tripartite model of working memory. The model emphasizes a multi-component model of working memory that includes specific mental structures that process mental representations corresponded by each of the senses.

Today, cognitive scientists recognize that humans perceive information through a diverse set of sensory organs; however, Baddeley and Hitch's model focused exclusively on the encoding and processing of visual and aural information. Importantly, the model acknowledges that information perceived via one of the sensory mechanisms may be transformed in working memory into a mental representation of a different kind. For example, information that is sensed via the ears in the form of spoken words can be re-represented in working memory as visual information: upon hearing the word "cat" a student may consider a mental image of a cat rather than consider the sound of the word itself (*47*). Similarly, upon seeing a visual picture of a cat, a student may consider the sound of the word "cat" to describe the image. As such, the auditory loop and the VSSP work synergistically to maintain and manipulate information for transfer to long-term memory.

The transformation of information between modalities in this way leads to specific predictions about learning and memory that have been empirically validated in multiple contexts. Among those predictions most useful to the chemistry education research community are those resultant from Dual Coding Theory. Proposed by Paivio (*50*) Dual Coding Theory predicts that any word or concept will be more easily learned and later recalled when it refers to a concrete object that can be mentally represented dually with a visual or pictorial image and a aural or verbal image. This theory has been validated in multiple experiments that examine how easily individuals can remember word lists (*51–53*). In the absence of any organizing principles, individuals more easily recall concrete nouns than abstract nouns. The tripartite model offers a causal explanation for this observation. Memorizing a list of spoken words requires the individual to first attend to aural information, which is encoded in an aural image. Thus, any words that can be re-represented with a visual image in the VSSP are more easily learned as both the visual image and the aural image are transferred together to long-term memory. Similarly, the learner can access either the visual or the aural image, which increases the accuracy of recall at a later time given multiple avenues to access the information. Conversely, this model predicts that any abstract concepts that cannot be dually (or multiply) represented in working memory will be both more difficult to learn and more difficult to recall.

The tripartite model of working memory also predicts that learning and later recall are negatively affected by (1) the amount of information presented at a given time, (2) attentional interference, and (3) similarities among mental representations that refer to different information (*46*). Each of these predictions rests on the model's assumption that working memory has a limited capacity (*54*). Thus, when learners are tasked with memorizing large amounts of information that exceed working memory capacity, they are unable to maintain this information in working memory effectively (and therefore unable to transfer that information to long-term memory). Similarly, when learners are placed in situations that put competing demands on their attentional resources, working memory capacity is exceeded. For example, when learners are required to attend to large amounts of visual information, the VSSP can maintain only a small portion of the visual information at any given time. Finally, memorization and recall are impeded in instances where learners are tasked with using the same mental representation to refer to multiple pieces of information. In these cases, error rates are increased as the possibility arises for the learner to recall the correct representation, but associates that representation with the wrong meaning. For example, recall errors are higher when learners are tasked with memorizing lists of words with similar sounds, but different meanings.

Implications of the Tripartite Model of Working Memory

The tripartite model of working memory motivates CER research paradigms that narrowly examine how students perceive, encode, and recall the various representations used in chemistry visualizations. The model supports investigations that seek to identify which representations are most effective, which representations are (in)effectively paired, or how students encode molecular representations. Moreover, the model is best applied to experimental designs that consider (1) the amount of information presented at a given time in a visualization, (2) the presence or absence of attentional interference in the learning environment, and (3) the typological and topological similarities among representations that support or inhibit dual coding (*55*). Notably, the tripartite model offers little guidance to those researchers investigating how visualizations improve conceptual understanding or affect in the chemistry classroom. As above, the model is exclusively concerned with how information is encoded, stored, and recalled.

The tripartite model of working memory also offers multiple implications for the design of animations and simulations in chemistry. First, the model suggests that visualizations can overcome a primary challenge to learning chemistry. Namely, the majority of concepts and processes that students learn about in chemistry do not correspond to any phenomena that students can visually perceive. When faced with learning about an idea as simple as an "atom," students are limited to representing this idea in the auditory loop as nothing more than a word and its corresponding definition. Thus, animations or simulations that provide visual representations of atoms address this challenge simply by providing students with a concrete representation that can be encoded in visual working memory. Similarly, visualizations that offer visual representations of quantitative relationships are equally likely to lead to improved retention and recall. Simulations that demonstrate the relationships between quantitative variables using dynamic plots coupled to an animation of molecular interactions offer multiple visual representations that can be linked together with an aural representation of mathematical formulas. For example, visualizations can help students to mentally represent Boyle's Law visually in terms of collisions between particles and an expanding container, visually in terms of a function plotted on a graph, and aurally in terms of a mathematical expression.

These implications result in two clear design principles. First, the model cautions against using one representation for multiple concepts because this increases the likelihood that students will confuse those concepts at recall due to a similarity effect. Thus, designers should strive for a high degree of representational consistency in their designs to support learning. For example, designating a specific shape and color for an element will help students to associate one image consistently with that element. Second, the model motivates the use of explicit feedback to help students make connections between multiple representations of a phenomenon that is represented on multiple levels. Students are rarely able to perceive the correspondences among multiple representations or associate multiple representations meaningfully when they are displayed simultaneously (*12*, *56*). Learning environments that help students identify the relationships among multiple representations are likely to improve the encoding of each representation and its later recall (either alone or together with other representations). Without explicit feedback students are less able to perceive the relationships between different representations. Notably, empirical questions remain outstanding regarding the relative benefits of the amount and type of feedback and the limitations of representational consistency.

The "Knowledge-in-Pieces" Model of Conceptual Change

Whereas information processing models offer narrow predictions about retention and recall, they have little to say about the quality of conceptual understanding or complex problem solving. In contrast, *conceptual change models* focus on the knowledge structures that learners develop from their experiences whether in formal learning environments or everyday life (*57*). In this way, conceptual change models are more agnostic about the structure of the mind and do not make strong claims about the location of information in memory or the processes involved in retention and recall. All conceptual change models focus on the processes by which learners integrate information to develop coherent (and incoherent) understandings of the world (*58*, *59*). As such, conceptual change models account for a student's knowledge before and after instruction with analyses that both supplement and extend those of information processing models.

Conceptual change models vary in the extent to which they focus on processes of *accretion* and *change* that transform knowledge structures. Importantly, these processes are different in kind and each conceptual change model accounts for them in different ways. Most models do not consider the processes involved when students enrich their understanding by "adding new knowledge or gap filling incomplete knowledge" (*59*) through accretion. These instances of learning are considered fairly trivial: given the lack of conflicting information, students have only to add new information into their existing knowledge structures. Instead, most conceptual change models attempt to account for the processes involved when students must actively modify their understanding upon encountering information that is in direct conflict with existing ideas.

Today, cognitive and learning scientists actively debate the validity of multiple competing models of conceptual change that vary significantly in their underlying assumptions about the nature of knowledge and the processes involved in conceptual change (see (*60*, *61*) for recent examples of this debate.). In our opinion, three models are at the center of this debate: models that focus on mental model revision (*62*, *63*), models that focus on ontological recategorization (*59*, *64*) and the "knowledge-in-pieces" model (*37*, *38*, *65*, *66*). These models

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offer contrasting predictions about the efficacy of various interventions for promoting conceptual change; however, all three models posit that conceptual change is more complicated than simple belief revision. That is, each model asserts that conceptual change necessarily involves the revision of false ideas, or "misconceptions," to scientifically correct models; however, each model also asserts that belief revision is not sufficient to explain the failure of students to apprehend scientific concepts, the striking persistence of misconceptions despite years of science instruction, or the genesis of novel misconceptions while learning. We believe that each of these models can provide useful explanations for the efficacy of visualizations as well as precise design principles; however, we suggest that the *"knowledge-in-pieces" model (KiP model)* offers the most utility for chemistry education researchers working on the development of new animations and simulations at multiple levels of instruction.

The chemistry education research community has devoted considerable effort to identifying the misconceptions that students have regarding fundamental domain concepts *(e.g.,* (*67–75*)*)*. Indeed, a large number of reports are available that document student (and teacher) misconceptions, and researchers actively study the prevalence of chemistry misconceptions among different populations. While such efforts have been instrumental helping the community target which concepts new interventions should address and when they should be implemented in the curriculum, they offer little in the way of helping us understand why these concepts are difficult to learn and why some chemistry misconceptions are intransigent. Such work has motivated design principles that advocate instructional methods that elicit, confront, and eliminate misconceptions, which have seen little success in learning environments with or without accompanying visualizations. Contemporary conceptual change models are increasingly common in chemistry education research *(e.g.,* (*76*, *77*)*)* and we believe that researchers designing and studying new visualizations would benefit greatly from adopting these models in their work.

Features of the Knowledge in Pieces Model of Conceptual Change

In contrast to other conceptual change models, the KiP model of conceptual change most closely focuses on the dynamic construction of explanations in the moment and, in our opinion, provides the most coherent explanation for the complexity of conceptual change in disciplines where students lack significant experience with domain concepts prior to instruction. Many concepts that students encounter in the chemistry classroom are not clearly grounded in everyday experience, and students are left to bootstrap their understanding at many levels of instruction. Thus, conceptual change models that do not focus on both the processes of accretion and change cannot account for the genesis of new misconceptions while learning chemistry. For example, students erroneously believe that chemical equilibrium occurs when the concentration of two substances become equal (*67*, *78*). Prior to instruction, students are unlikely to hold any coherent beliefs about the concept of chemical equilibrium that would conflict with the accepted definition. Nevertheless, the KiP model can account for this misconception by analyzing how students integrate prior

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knowledge from outside traditional disciplinary boundaries to construct dynamic (mis)understandings in the moment.

The KiP model of conceptual change arose in response to extant conceptual change models that include a single process: the elimination of misconceptions followed by replacement with scientifically acceptable concepts. In 1993, diSessa and colleagues proposed a model of conceptual change that abandoned the idea of "elimination and replacement" in favor of a model that included a knowledge system "with numerous elements and complex substructure that may gradually change, in bits and pieces and in different ways" structures (*37*). The authors noted that traditional conceptual change models at the time were inconsistent with empirical evidence that learning involves the integration of new information with existing knowledge and that prior knowledge plays an instrumental role in shaping a student's developing understanding. To address this criticism, diSessa's knowledge-in-pieces model privileges the role of prior knowledge in conceptual change and frames meaning making as a dynamic process that involves coordinating existing knowledge with new knowledge in ways that are highly sensitive to contextual factors. From the perspective of the KiP model, a "misconception" is more complex than a simple false or inaccurate statement. Rather, what we label as misconceptions are instead rationale explanations that students produce in the moment as knowledge elements coordinated in different ways.

As a constructivist theory, the KiP model argues that learning involves both the accretion of new knowledge elements and the reorganization of knowledge elements as the learner attempts to integrate new information with existing knowledge concepts (*66*, *79*, *80*). Thus, students are seen to bring with them a wealth of ideas from their everyday experiences with which they bootstrap their understanding of unfamiliar abstract science (*81*, *82*). In some cases, these ideas contribute effectively (e.g., what students know about force and motion from everyday life is highly relevant to physics learning). In other cases, students use ideas to gain purchase on unfamiliar concepts in ineffective ways (e.g., many students rationalize that air is not matter because it is invisible). Regardless of how these knowledge elements influence a students' developing understanding, the KiP model stresses that researchers must account for how they influence learning whether by accretion or reorganization.

The KiP model of conceptual change is ambiguous with regard to the size and quality of the knowledge elements at play in the knowledge system in favor of analyzing the processes involved in conceptual change (*37*, *65*). However, among the various knowledge elements proposed by KiP researchers, one particular element, the *phenomenological primitive*, is particularly relevant to the design and study of animations and simulations for teaching chemistry. Posited in 1993 by diSessa, phenomenological primitives (i.e., p-prims) are unstructured knowledge elements that contribute to a student's intuitive knowledge of physics. P-prims are relative small knowledge elements that develop from "superficial interpretations of experienced reality" (*65*), and permit student's to make reliable and productive explanations of the physical world. Importantly, p-prims are not modeled as coherent beliefs; rather, p-prims are abstractions developed from systematic experiences that help students to interpret the physical world. When contextual factors cue the activation of a p-prim, it is highly likely to influence the quality of a student's explanation in the moment or their developing understanding.

As noted, the granularity and structure of p-prims or other knowledge elements is of secondary importance to the role that they play in conceptual change. As students participate in formal science instruction, those knowledge elements that have proved fairly reliable in everyday meaning making may become integrated into developing knowledge structures together with accepted scientific information. Consequently, these knowledge elements are activated together dynamically across various tasks and result in observed "misconceptions." For example, a student who appears to hold the misconception that "equilibrium reactions are static" may instead by employing the "canceling" p-prim. The "canceling" p-prim is an abstraction that opposing forces act in equal and opposite ways and thus cancel each other. Applied to the concept of chemical equilibrium, "canceling" would lead a student to conclude that forward and reverse reactions stop when equilibrium is reached. Although much work has been devoted to the role of p-prims in intuitive physics, recent work by CER researchers has demonstrated an influential role of p-prims in chemistry learning (*19*, *83*, *84*), and additional studies are needed to understand how such knowledge elements influence learning with visualizations.

The KiP model suggests that conceptual change is best promoted in learning environments where students are provided with opportunities to reflect on their prior knowledge, engage in extended activities that allow them to integrate new information with their prior knowledge, and reflect on how their understanding has been revised (*37*). Thus, the KiP model offers two reasons why learning environments that do not include these features typically result in poor conceptual change. First, when prior knowledge is not elicited and reflected upon, problematic knowledge elements may be integrated tightly with the target learning objectives to produce observed misconceptions. Second, learning environments that emphasize the identification and elimination of misconceptions through confrontation rather than revision are unlikely to promote conceptual change. Such environments are predicated on the false assumption that misconceptions can be eliminated and thus fail to provide students with compelling reasons to revise their existing ideas that rest on years of experiential evidence.

Implications of the Knowledge in Pieces Model of Conceptual Change

Unlike information processing models, the KiP model attributes no inherent benefit to the visualization itself; rather, the model suggests that the benefit of visualizations results from how they are used to help students relate their current understanding with accepted scientific ideas. Thus, visualizations designed with the simple goal of "showing" molecular interactions are unlikely to result in any lasting conceptual change. Instead, conceptual change is promoted in learning environments that ask students to systematically compare their observations from a visualization with their prior understanding. Moreover, such environments must acknowledge that conceptual change is unlikely to result from a single exposure to a visualization. As conceptual change is a gradual process, students need repeated opportunities to explore a visualization before any productive conceptual change is expected. Without allotting time for gradual revision of understanding, students will demonstrate accurate understandings only immediately after instruction (*37*, *65*).

The knowledge-in-pieces model suggests that CER researchers recognize students' prior knowledge as a productive resource rather than an obstacle to be eliminated or ignored (*37*, *65*, *66*, *85*). Thus, new research agendas that include visualizations must characterize the quality of students' conceptual understanding not only before and after instruction, but also *during instruction*. Thus, the KiP model can be employed to identify which visualizations best take advantage of prior knowledge, how student meaning making changes with access to visualizations, and how visualizations best help students capitalize on their knowledge resources. Research paradigms that explore such questions must include microgenetic approaches to analyze student understanding and learning with visualizations and identify individual differences among students (*80*). Research paradigms that attempt to compare achievement differences between groups of students who do or do not use visualizations are unlikely to yield data that inform questions about conceptual change in chemistry.

The KiP model offers several implications for the design of learning environments that use visualizations. Notably, the model has little to say about the modality of representations used in a visualization or interface design. Instead, the KiP model offers CER researchers three design principles that focus on how visualizations should be used in novel learning environments. First, visualizations should be embedded in activities that elicit prior knowledge and provide as many opportunities as possible to compare that knowledge to their developing understanding. Such environments position students to compare their current understanding with information presented in a visualization to scaffold knowledge revision as opposed to misconception elimination. Second, visualizations should systematically provide students with explicit feedback on the quality of their understanding at multiple points during a learning activity. In this way, visualizations can be leveraged as a resource to help students evaluate the quality of their developing understanding in real time. Third, visualizations should be embedded in microworlds that offer students freedom to explore "wrong ideas." As above, students are likely to bring with them many "wrong ideas" that can be leveraged to promote conceptual change. By allowing students to explore those ideas, teachers can gain important insight into what knowledge elements students are bringing to bear in a lesson and provide more targeted feedback to promote conceptual change.

Social Cognitive Learning Theory

New visualizations embedded in learning environments provide increased opportunities to capitalize on student-student and teacher-student interactions in the chemistry classroom. The tripartite theory of working memory and the KiP model of conceptual change both offer important insights into the challenges

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students face learning chemistry and offer specific recommendations for the design of visualizations to help address those challenges. Of note, both models focus narrowly on the individual learner as the unit of analysis and leave the social interactions afforded by these learning environments unanalyzed. Although researchers who employ the tripartite model or the KiP model have acknowledged the important role of socio-contextual factors in learning, neither model attempts to account for how those factors influence recall or conceptual change. Thus, neither model can fully account for the success or failures of visualizations employed in classrooms or other authentic settings that involve students learning together with a teacher. To address this limitation of both models, we review the potential of *social learning theories* to inform research on the design and efficacy of visualization tools in chemistry.

Although the first social learning theories originated in the late 1800s with Vygotsky's early writings, theories that focus closely on the role of social interactions in learning did not rise to prominence until the late 1970s and early 1980s. Prior to that time, behaviorist and cognitivist theories dominated research on human learning with exclusive focus on the individual learner as the unit of analysis (*86*). Social learning theories received attention after the fall of behaviorism and rise of cognitivism as scholars became increasingly dissatisfied with the failure of extant theories to account for the role of social interactions. These scholars agreed with cognitivists who rejected behaviorist learning principles; however, unlike cognitivists they argued that a comprehensive model of human learning must move beyond a narrow focus on the individual. Among the most common theories employed in the cognitive and learning sciences community today are Vygotsky's Theory of Social Development (*87*, *88*), Lave's Situated Learning Theory (*89*), and Bandura's Social Cognitive Learning Theory (*90*).

Although there are important distinctions between each of these theories, we do not see them as competing in the same way that conceptual change and information processing models compete. Rather, each theory attends more closely to different aspects of the social environment and yields convergent perspectives on human learning and development. Collectively, social learning theories attempt to analyze learning as a process that occurs between teachers and students as well as among individuals. Thus, each theory places an emphasis on the active role of social agents (and cultural factors more broadly) and frames learning as a process rather than an outcome. Among these three theories, we believe that Bandura's *Social Cognitive Learning Theory* is the most empirically supported theory that offers the most utility to the chemistry education community.

The chemistry education research community has long recognized the important role of social interactions in the classroom, and we believe that researchers working on the design of new learning environments should capitalize on that tradition. CER researchers have made extensive use of Vygotsky's work to research learning obstacles in the chemistry classroom and to motivate the design of new learning environments (*91*, *92*). Using a Vygotskian approach, these researchers have foregrounded how teachers and peers can extend the capabilities of a student to achieve greater levels of understanding and performance than the student would otherwise achieve alone. Although we concur that Vygotskian

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perspectives have excellent utility for understanding the role of environmental factors in student learning, we do not believe Vygotsky's Theory of Social Development offers precise accounts for the causal role of visualizations in learning chemistry or offer clear design principles for their use. Similarly, Lave and Wenger's (2003) model of situated learning offers strong insights into the social practices that characterize chemistry as a discipline, but offers few recommendations on the design of learning environments that use visualizations.

In contrast, we argue that Bandura's (1977) Social Cognitive Learning Theory offers a more precise model of the role of social agents in human learning and a clearer bridge to conceptual change and information processing models of learning. Social Cognitive Learning Theory builds on prior cognitivist perspectives and offers a model of learning that attempts to analyze how individuals learn within a social context. Thus, social cognitive learning theory does not downplay the analysis of mental representations: the theory attempts to explain how social factors play an active role in helping an individual learner to construct mental representations while learning. To that end, social cognitive learning theory directly addresses the role of motivation and human agency in learning in ways that other social learning theories do not. Because of this, the theory provides a model for research on visualizations and offers design principles for curricular structure and pedagogical methods. Indeed, social cognitive learning theory underlies several research programs among cognitive and learning scientists studying learning in authentic contexts *(e.g.,* (*93–95*)*)*, and it offers many recommendations to the CER community.

Features of Social Cognitive Learning Theory

Bandura proposed social cognitive theory to address what he perceived as a fundamental failure of information processing theories advocated by cognitive scientists (*90*). Namely, Bandura argued that these theories, which approximated the human mind to nothing more than a biological calculator, were flawed since they did not acknowledge that humans are social animals that exercise a degree of control over their own behaviors and their environment. He contended that cognitivist information processing models could only partially explain how humans acquired, retained, and recalled information and offered a theory that rejects the premise that human cognition and learning is best modeled as disconnected from the brain and environment. In contrast, social cognitive learning theory attempts to model learning as a social process that is directly affected by situational and environmental factors. As Bandura (*40*) argued, "Of the many cues that influence behavior, at any point in time, none is more common than the actions of others" (p. 206).

In brief, social cognitive theory posits three central tenets: (1) human learning is agentic, (2) attitudinal factors play a critical role in one's willingness to learn and the quality of learning, and (3) learning is promoted through social interactions. Social cognitive learning theory analyzes the actions of an individual learner as a part of a larger system that includes social and environmental factors

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that operate reciprocally within a larger cultural context. Like the KiP model, the social cognitive theory models learning as an active process that involves more than "just exposure to stimulation, but agentic action in exploring, manipulating, and influencing, the environment that counts" (*86*). Accordingly, learners are viewed as active agents that execute intentional (as opposed to responsive) behaviors to achieve self-defined goals. Moreover, the model of the learner as agentic is invariant across contexts. Whether a student is sitting quietly in a lecture or moving actively through a laboratory procedure, social learning theory views the learner as an active agent.

Agency is characterized by several cognitive activities that define the learning process 86. First, learners establish learning goals that, when achieved, result in increased feelings of self-worth or an improved self-concept. Second, learners exercise forethought and develop plans of action that will facilitate goal attainment. With goals and a plan of action in hand, learners execute strategies to both motivate and regulate their activities. Finally, learners engage in reflective strategies to evaluate how effectively they are meeting their goals. Agency is promoted under situational and environmental conditions that promote a high degree of efficacy. That is, learning is optimal when individuals perceive that they are able to establish clear goals and exercise control over the actions that lead to goal attainment. Those learning environments that do not permit learners to exercise control decrease agency and result in disaffection and decreased motivation.

Outside of the classroom, social learning theory also accounts for the ways in which cultural and societal factors can shape learners' self-concepts and influence their goal setting behavior in academic settings. Most commonly, social learning theory has been used to explain the educational achievement gap between different groups of students (*40*). According to the theory, children actively construct self-concepts that are influenced by cultural stereotypes about who can and cannot be academically successful. These stereotypes may promote or inhibit children's perceived efficacy in a domain and thus influence planning and goal setting behaviors. For example, girls who grow up in societies that promote deficit models of women in science may develop self-concepts that do not include science-related identity constructs. In such a cultural environment, girls perceive that they have little control over their science learning, perceive themselves to have low efficacy in science, and ultimately avoid science studies.

In addition to claims about the role of attitudinal factors and agentic processes of the individual, social cognitive learning theory also accounts for learning through social interactions (*40*). Specifically, social learning theory posits that learning is promoted in settings where learners are able to observe the motivations, intentions, and behaviors of others through *social modeling* (*86*). Importantly, not all observations lead to effective learning. Social modeling is most effective in those situations where the learner attends to the actions of the modeler, retains that information, and reproduces the observed behaviors. Social learning theory has little to say about the underlying structure and process of attention, retention, and reproduction; however, the important insight of Bandura's theory was that humans are able to learn readily by simply observing the activities of other humans regardless of any observable changes in the learner's behavior.

Implications of Social Cognitive Learning Theory

The central tenets of social modeling theory lead to three implications for the design of learning environments (*40*, *90*). First, learning is promoted in environments where students are able to exercise control over the learning to attain clearly defined learning goals. Curricular and instructional methods must help students articulate those learning goals and develop plans of action that will permit the student to reach those goals. Second, learning is promoted in environments were goal attainment promotes improved self-concepts. Methods that include demoralizing students or curricular activities that do not have clearly defined goals produce apathy and frustration among learners. Finally, learning is promoted in environments where instructors or peers make their intentions and plans of action visible to students to support observational learning. Moreover, learning environments where students are able to reproduce the instructors' behaviors in order to receive constructive feedback can help students develop self-regulating behaviors.

Social cognitive learning theory suggests research agendas that focuses on how students learn with visualizations together and how students learn from teachers who model their thinking using visualizations. Unlike the previous models presented in this chapter, social cognitive learning theory emphasizes the role of social interactions in the classroom and broader societal and cultural factors. Such work involves analyzing changes in individual learning as a result of social factors or the quality of social processes in classrooms that employ visualizations. Thus, research paradigms that make use of the model might study how visualizations can promote meaningful social interactions, how teachers can use visualizations to effectively model their thinking, and how visualizations can promote self-efficacy and agency. Research designs that address these questions might include discourse or interactional analyses or experimental designs, such as those employed by Bandura himself (*86*, *96*).

Two clear design principles result from the application of social cognitive learning theory to chemistry visualizations. First, the theory suggests that visualizations should be used in ways that promote interactivity among students and teachers. In this way, teachers and peers can use the visualization as a resource to model their thinking and help students learn through observation of others (as opposed to working with a visualization in isolation). As such, the visualization is conceived of as a resource with which teachers can better model their thinking. Second, visualizations should offer students a high degree of control. In this way, students can perceive that they have control of their learning, which will promote self-efficacy and agency. Students are likely to see visualizations that offer little control as environments in which they are unable to influence the progress of their own learning.

Conclusion

Among the sciences, chemistry is the discipline that relies most on visualizations for communicating both in teaching and in practice (*97–99*).

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As such, the CER community increasingly advocates for the use of novel visualization technologies at all levels of instruction. Despite the enthusiasm of these technologies among researchers, teachers, and students, few studies have demonstrated that visualizations reliably improve student learning or attitudes toward chemistry. In this chapter, we have argued that the failure of many visualization tools is due, in part, to their unprincipled implementations in the classroom. Too often, our confidence in the beneficial affordances of visualizations, have led us to assume that they are useful in any context because they help students "see" the chemistry appreciated by experts. In contrast, we suggest new research programs that involve the design and implementation of visualizations should assume a skeptical stance. Moreover, we urge the CER community to employ theoretical frameworks employed extensively among cognitive and learning scientists.

To that end, we have reviewed three contemporary models of learning from the cognitive and learning sciences communities that offer diverse explanatory models for the potential of visualizations. First, we discussed the potential of information processing theories to explain the mechanism by which learners encode, store, and recall knowledge representations. Specifically, we outlined the memory structures and processes described by the tripartite model of working memory (*35*) and the implications of the model for the design of chemistry visualizations. This model, with its narrow focus on memory, offers important implications for the design of visual representations and their embedding in multi-representational displays. Indeed, the model serves as the foundation for contemporary theories of multimedia design *(e.g.,* (*47*)*)* and we believe the CER community would benefit greatly from employing the tripartite model to research the design and efficacy of visualizations in chemistry.

Second, we reviewed the knowledge-in-pieces (*38*) model of conceptual change to motivate research paradigms that examine the role of visualizations in improving students conceptual understanding. Unlike the tripartite model of working memory, the knowledge-in-pieces model offers few recommendations regarding the design of visualizations per se. In contrast the model has strong implications for the design of learning environments and pedagogical methods that make use of novel visualizations. Importantly, this model offers an explanation for how well-designed visualizations can fail to stimulate conceptual change when they are embedded in learning environments that do not provide students an opportunity to reflect on their prior knowledge while learning.

Finally, we presented social cognitive learning theory (*40*, *90*) as a model to examine the causal role of social interactions when learning from visualizations. Social cognitive learning theory characterizes an individual's learning process against local, social, and situational factors as well as broader cultural factors. The theory cautions us against assuming that new visualizations strongly motivate students to learn. Rather, visualizations provide new opportunities for teachers and students to model their thinking in the chemistry classroom and support observational learning. More broadly, social cognitive learning theory suggests that visualization technologies are unlikely to address societal factors that shape student attitudes toward chemistry independent of the manner in which teachers employ them in the classroom.

Our goal with this chapter has been to stimulate designers and researchers to reflect on the utility of various theoretical frameworks that account for the efficacy of visualizations. We have suggested that models of learning more commonly employed outside of our traditional disciplinary boundary may offer new perspectives and directions for research on chemistry visualizations. In fact, we would argue that a CER researcher with strong disciplinary expertise and pedagogical content knowledge can leverage one or more of these models to produce a more rigorous and informative research program on the efficacy of visualizations than any expert working outside chemistry. Regardless of the models we use to motivate and situate our work, we must remind ourselves that it is not enough simply to know whether visualizations are effective. The more important task at hand is to understand why they are effective for improving student learning in our discipline.

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Chapter 3

Designing and Implementing Effective Animations and Simulations for Chemistry Learning

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With recent advances in technology, animations and simulations are increasingly available for science education. These dynamic resources can be useful for communicating some of the critical ideas that are fundamental to chemistry; however, numerous factors contribute to their effectiveness. In this chapter, we describe our research in designing and implementing a sequence of interactive multimedia simulations on Kinetic Molecular Theory and associated topics, developed for use in high school classrooms. We first discuss the role of representations in chemistry learning, specific attributes of simulations and animations, and theoretical approaches to how people learn from multimedia resources in general and dynamic representations in particular. We then situate this theoretical discussion in practice by describing our own experience in designing, building, testing, and implementing simulations for chemistry education.

Dynamic Representations and Science Making

Recent advances in computer technology have made simulations and animations an increasingly available resource for science education. For the field of chemistry in particular, *dynamic representations*, which can incorporate motion and change, provide a means to help students visualize concepts, phenomena and

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processes that are critical to comprehension, yet not easily represented in static textbook diagrams or by traditional classroom visual aids (*1*, *2*). Over the past eight years, our multidisciplinary team has designed, developed and implemented a sequence of simulations on kinetic molecular theory and associated topics aimed at high school chemistry students. In our team approach, each expert—including cognitive scientists, developmental psychologists, instructional designers, science educators, and chemists—brings a uniquely informed perspective to the design, development, evaluation, and integration of these materials. Our research, which we describe in this chapter, has supported us in making a number of design decisions about specific features of animations and simulations that can have a positive effect on student learning. We begin the chapter by discussing the role of representations in chemistry learning and the specific attributes of animations and simulations. We then outline theoretical approaches that address how people learn from multimedia applications in general and dynamic resources in particular, and lay out a set of principles that can inform the design of animations and simulations to support chemistry learning. Finally, we situate this theoretical discussion in practice by describing our own experience in designing, building, testing, and implementing simulations for chemistry education.

Representations in Chemistry Learning

For centuries, educators have been intrigued by the power of visualizations to express ideas that are not easily communicated by words alone (Figure 1). In science education as well as science practice, visual representations such as photos, diagrams, graphs, animations, and simulations serve a number of functions. For example, they can depict explanatory processes that are otherwise not observable, such as molecular models (*3*); display abstract conceptual material in a visual format (*4*); or present an organized array of data or other complex information ((*5*); Figure 2).

Figure 1. "Geometrician measureth the height of a Tower". Reproduced from reference (6).

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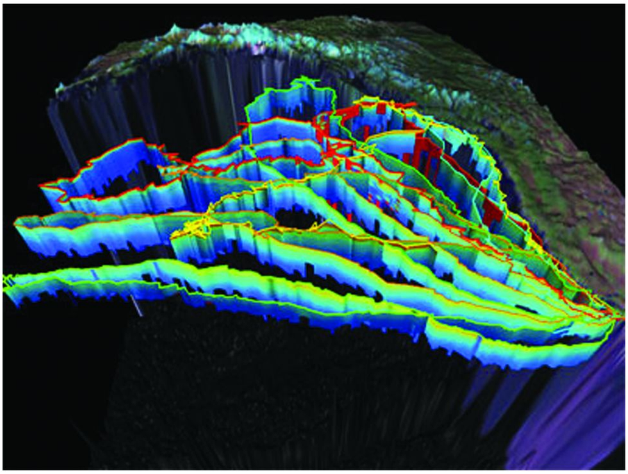

Figure 2. Visualization of ocean temperature profiles generated by traveling seals. Image courtesy of Dan Costa, UC Santa Cruz, reference (7).

For practicing scientists, visual representations play a central role in the generation of new scientific knowledge (*8–10*), functioning as tools with which to reason about problems and solutions as well as collaborate with others (*11*). For science learners, too, appropriate representations can not only convey information, but may support active learning by giving students the opportunity to discern patterns through their own investigation (*12*).

In the study of chemistry, visual representations can be particularly valuable given that processes at the molecular level are impossible to observe by direct methods (*11*). However, the fact that both motion and change are critical components in explaining particulate phenomena can make the design of representations quite challenging. A diagram depicting a dynamic chemical process such as phase change, for example (Figure 3), may seem rather daunting to a novice in the field of chemistry.

To complicate matters even further, a nuanced understanding of chemistry relies on three distinct but interconnected levels of representation: the macroscopic, or observable level; the sub-microscopic, or particle level; and the symbolic level, including chemical symbols, formulas, and graphs (*14*). One of the central goals of chemistry education is to assist learners in navigating between these different types of representations. This challenge was noted by Peter Atkins in a plenary lecture to the International Conference on Chemical Education, in which he highlighted the difficulties of communicating chemistry to students (*4*). Atkins described chemistry education as the bridge between the macroscopic observable field and the explanations of these observations, which exist in the realm of the sub-microscopic level. He argued that the need for abstraction—that is, the ability to conceptualize molecules, atoms, entropy, enthalpy and relationships between variables—is both essential and pervasive in chemistry, and that the use of specific visualizations to support abstract thinking should suffuse the learning and teaching of chemistry.

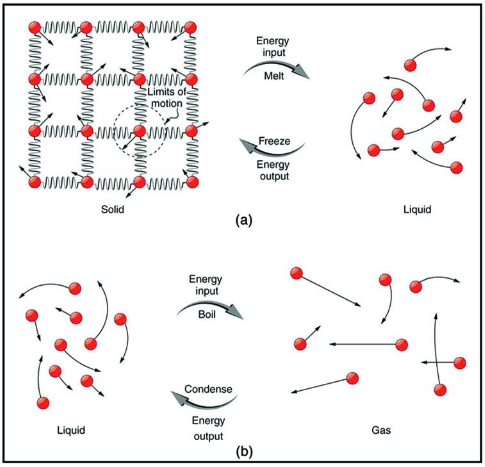

Figure 3. "(a) Energy is required to partially overcome the attractive forces between molecules in a solid to form a liquid. That same energy must be removed for freezing to take place. (b) Molecules are separated by large distances when going from liquid to vapor, requiring significant energy to overcome molecular attraction. The same energy must be removed for condensation to take place. There is no temperature change until a phase change is complete.", and http://cnx.org/content/m42225/1.6/. Reproduced from reference (13), which can be found at http://cnx.org/content/m42225/1.6/.

Given this array of challenges and goals, the potential of dynamic multimedia resources to support visualization in science education seems promising. Because animations and simulations of chemical processes at the molecular level can incorporate both motion and change, they may afford unique opportunities for clear representation of complex concepts. In a report to the National Science Foundation, the Molecular Visualization in Science Education Workshop (*15*) argued that a major strength of computer visualization is its capacity to represent causation more vividly, dynamically, and accurately than has traditionally been possible.

Animations or simulations of system behavior may help learners to interpret concurrent changes in variables by revealing an underlying computational model (*16*), and embedded signaling or guidance can scaffold the learner's successful use of a multimedia resource by directing attention to relevant points (*17–19*). Dynamic visualizations have the capacity to present multiple modes of representation that are simultaneously displayed and interactively linked to clarify the connections between them (*2*). For example, as rising temperatures in the representation of an ideal gas cause volume to increase, an associated graph can update to record these changes (Figure 4). However, dynamic representations may present challenges as well as benefits for learning (*20*, *21*). In order to examine the issues posed by the use of animations and simulations, we must first consider the features that characterize and distinguish these two types of dynamic representations.

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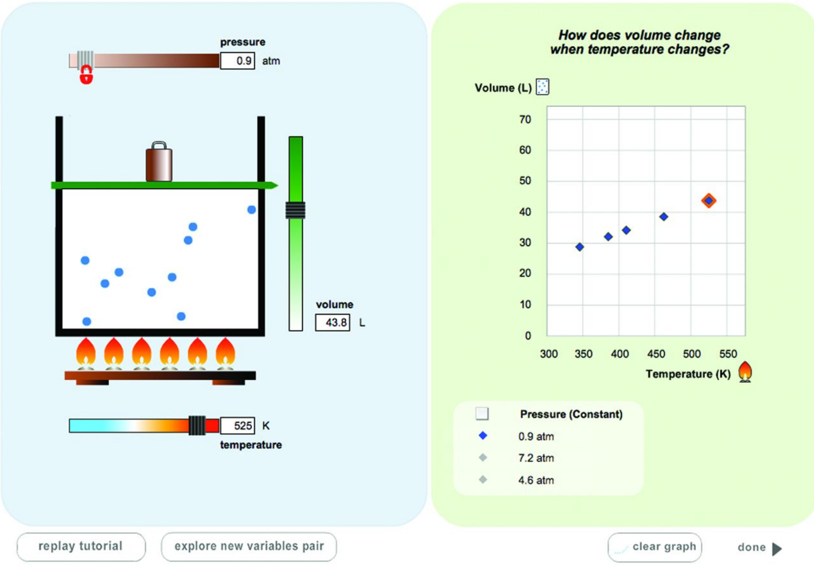

Figure 4. Temperature and volume changes within a dynamic model (left panel) appear on an interactive graph (right panel). (see color insert)

Animations and Simulations

What distinguishes an animation from a simulation? In general, animations are representations that involve change over time (*22*), created by generating a series of images or frames (*23*). In the context of science education, an animation may depict a process or phenomenon in real time, slow motion, or visualized from different points of view; it may also present abstract information such as a change in pressure or the relationship between two variables (*24*). Animations may include scaffolding, such as visual cues, to draw the viewer's attention to specific features, and may incorporate interactivity, allowing the user to stop, start, or repeat portions of the presentation. Weiss, Knowlton, and Morrison (*25*) outline five different functions of animations: to make instruction attractive; to promote attention; to motivate learners; and to present or clarify information.

A simulation is a special case of interactive animation that presents a phenomenon, process, or system which a user can explore by manipulating various parameters (*26*). In using a simulation, the user is able to generate hypotheses, adjust variables within the virtual environment, and observe the effects of the manipulation. Underlying any simulation is a model that governs how the system responds to user input, and it is through the resulting interactions that the user may arrive at a conceptual understanding of that model (*27*, *28*). Rieber (*28*) suggests that animations focus on presenting scripted *explanations* of information, while simulations emphasize *exploration*.

Simulations can take a number of forms. For example, a simulation might present a realistic representation of a chemistry lab. In this virtual environment, the user might be asked to select an on-screen beaker filled with a specific chemical, add an indicator, and observe the reaction to test whether the chosen chemical was an acid or a base (e.g., http://chemcollective.org/vlab/98). Another simulation might depict a real-world context such as a busy street, allowing the user to investigate a phenomenon such as pollution emissions by selecting various temperatures and varying weather conditions (e.g., http://www.smogcity.com/). On the other hand, rather than presenting a realistic situation, a simulation might involve an abstract idealized representation, such as the container of moving particles and associated graph pictured above (Figure 4). Simulations of this type afford the representation of forces and processes that are not normally visible in the natural world, such as vectors, as well as symbolic representations of those phenomena (*29*). The capacity of simulations to support learners in visualizing explanatory models is probably one of the most compelling educational justifications for their use. In general, dynamic representations can serve to support learners in retaining factual information (*recall*), in comprehending information (*comprehension*), or in applying new information to a novel situation (*transfer*) (*30–32*). In the following sections, we contextualize the question of how animations and simulations can best be designed to benefit learners by giving an overview of learning with multimedia, and then discuss the special case of dynamic representations.

Learning with Multimedia

Over the past half-century, the consideration of visual representations in education has progressed from discussions of delivery mechanisms such as blackboards, filmstrips, and motion pictures (*33*) to an academic discipline that investigates the use of multimedia resources based on a learning sciences perspective (*34*). How do people learn from multimedia resources? What is the relationship between the design of such resources and the way in which people learn? In order to address these and other related questions, researchers have conducted numerous studies examining various aspects of multimedia learning, ranging from graphic design to learner characteristics and the incorporation of specific learning strategies. Key to all these investigations is the consideration of the role of cognitive capacity in learning and the consequent implications for the design and use of multimedia resources (*35*).

One approach that directly addresses cognitive capacity is Cognitive Load Theory (CLT) (*36*, *37*), which describes how information processing and the construction of knowledge are constrained by the limitations of working memory, or how much *cognitive load* the learner's cognitive system can bear. CLT defines three types of cognitive load. *Intrinsic* cognitive load relates to the inherent complexity of the material. *Extraneous* load is imposed by processing activities that are effortful, but not directly related to learning, such as the need

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to search for information on a poorly designed web page. *Germane* cognitive load refers to mental effort that the learner invests directly in comprehending the content material itself. These three types of cognitive load are considered to be additive. Due to the limitations of cognitive capacity, only a small total amount of information can be maintained or processed in working memory at any given time; excessive demands result in cognitive overload, which can impede learning.

The Cognitive Theory of Multimedia Learning, or CTML (*38*) complements Cognitive Load Theory in addressing the cognitive processes involved in learning with multimedia resources. Mayer defines *multimedia* as material that includes both sounds and pictures (*38*). The Cognitive Theory of Multimedia Learning rests on three key assumptions. The *dual channel assumption* suggests that humans perceive and process information in two separate channels, one for auditory/verbal information and one for visual/pictorial information (*38*, *39*). The implication of this assumption is that providing information through multiple channels may present an advantage for encoding and retrieval. The *limited capacity assumption*, closely related to Cognitive Load Theory (*37*), asserts that each processing channel has a limited capacity; a learner's working memory can retain only a small number of words or images at a given moment. Finally, the *active processing assumption* states that humans are not passive receivers of learning content, but rather must engage in active processing of incoming information in order to build mental models of new concepts. Such knowledge construction, according to CTML, occurs as a three-stage process: A learners must *select* relevant verbal and visual information from presented materials, *organize* the information to construct coherent verbal and visual mental representations, and *integrate* those representations with each other as well as with prior knowledge. Based on this model and on the key assumptions described above, CTML advances a set of principles for the design of multimedia materials. These principles address issues such as the combination of modalities through which information is presented, the arrangement of verbal and visual information in space and time, and the use of specific learning strategies. For example, the *redundancy principle* states that providing an excess of information may actually impede learning in a multimedia environment; this principle, like others proposed, has been validated by a number of empirical studies (see (*40*)).

Dynamic representations raise particular issues with respect to multimedia learning. Although, as noted above, such visualizations have the potential to enhance learning, they may also require significant mental effort for processing; their effectiveness is ultimately dependent on whether learners have the cognitive resources necessary to attend to and integrate the information provided (*19*, *37*, *41*). If a dynamic visualization includes multiple forms of representation that the learner must process, the cognitive capacity required to interpret and integrate those representations may exceed the available resources (*42*). Similarly, interactive functions incorporated into a resource in order to support learning often require the learner to plan and execute particular actions; these requirements may themselves impose a certain amount of cognitive load that can hinder as well as help learning (*35*). Another view suggests that though dynamic representations may sometimes be helpful, at other times they may actually impede learning by providing excessive instructional support for certain individuals (*21*). Schnotz and

Rasch (*21*) explain that non-dynamic representations require learners to perform their own *mental* simulations of dynamic processes or systems: If presented with a series of static diagrams illustrating sequential stages of a chemical process, for example, a student must invest significant cognitive effort to understand the progression from one diagram to the next. Some students would be incapable of this mental exercise, and for these individuals a dynamic representation may serve an *enabling* function by providing a dynamic model that would otherwise be inaccessible. Other students might be able to formulate a mental simulation, but only with difficulty, and at the cost of cognitive overload. For such a student, a dynamic representation might serve a *facilitating* function, alleviating some cognitive load so that more cognitive capacity is available for learning. However, for learners who have the capacity to generate a mental simulation on their own, a dynamic representation might serve an *inhibiting* function: Because the cognitive work involved in generating a mental simulation can be considered beneficial in helping learners to process and integrate information, a dynamic representation that effectively performs this mental work *for* students may actually reduce learning (*21*). In general, reviews of studies on computer-based learning environments have found that characteristics of both the learner and the task are critical determinants of learning outcomes in such environments (*19*, *43*, *44*).

Design Principles for Effective Dynamic Representations

As we begin our discussion of design principles for dynamic representations, it is important to specify several overarching assumptions. First, the Cognitive Theory of Multimedia Learning states that individuals learn more deeply from instructional materials that include both words and pictures rather than words alone. For chemistry education, we suggest that this is particularly important. Next, effective instructional materials must themselves have a coherent structure that will support the learner in constructing accurate mental models (*38*). Again, given the nature of the content to be learned in the domain of chemistry, this is critical. Finally, the limits of processing capacity play a significant role in the effective design and implementation of dynamic representations. Processing capacity is influenced by a number of factors including prior knowledge: Research on chess masters, for example, shows that an expert player looking at a chess game in play actually perceives more information than a novice (*45*, *46*). This means that a simulation or animation may be technically accurate, and seem perfectly clear to a chemistry teacher, yet include so much information that a novice cannot effectively process it. On the other hand, it is also important to bear in mind that not all learners are novices; the needs of advanced learners must also be considered. The *prior knowledge principle* in multimedia learning (*46*) suggests that advanced or expert learners may be impeded by techniques that aid low-level learners. Consequently, the individual characteristics of learners are an important factor in designing and selecting dynamic representations for educational use.

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The characteristics of a particular dynamic resource, of course, are also important. Dynamic representations can vary in the types of information and topics they present, as well as in their formats and objectives. However, they share three principal characteristics. First, they represent concepts visually as well as through text or narration. Second, they frequently incorporate some form of interactivity. Third, they integrate instructional tools and/or strategies, either explicitly or implicitly. Based on these three characteristics, we will consider *information design* principles, *interaction design* principles, and *instructional tools and strategies* that contribute to effective dynamic representations. Some of these principles apply equally to static representations and even non-digital materials, while others are specific to animations or simulations.

Information Design

Information design is concerned with selecting the modalities and formats in which information should be represented in order to facilitate comprehension. A key goal for effective information design is to avoid overloading a learner's cognitive capacity, which can be achieved by reducing extraneous cognitive load, described above. Research in multimedia has validated a number of principles that outline how visual and verbal information should be designed and combined within a multimedia learning environment.

Avoiding Split Attention: Spatial Contiguity, Temporal Contiguity, and Modality

As we have discussed, the capacity of working memory, in which information is held for processing, is strictly limited. When the learner must attend to and integrate essential information from several different types of input, the resulting split of attentional resources has implications for comprehension and retention (*47*). For example, if an animation is presented alongside an explanatory text that updates dynamically, the two sources of information compete for attention. If both sources are needed for comprehension, and each is relatively difficult for the learner to process, a split-attention effect ensues: Overloading working memory with these competing demands leaves few resources available for processing.

To address this issue, the *split-attention principle* suggests that multiple sources of information should be presented in an integrated format (*47*). For example, an early study of the split-attention effect in a computer environment found that students who learned programming skills from a paper-based manual that integrated all necessary information outperformed a second group who studied the same information, but had to switch between a paper-based manual and a computer (*48*). Several specific cases of the split-attention principle have been described, including the *spatial contiguity*, *temporal contiguity,* and *modality principles*. The *spatial contiguity principle* states that individuals will learn better when text and accompanying pictures are physically integrated on the screen, for example, by placing labels next to the appropriate objects rather than in a separate list. This practice reduces the necessity for visual search, which itself

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requires a commitment of cognitive resources. Similarly, the *temporal contiguity principle* states that words and pictures should be presented concurrently rather than consecutively, reducing the cognitive burden imposed by the need to hold one type of representation in working memory for an extended period before having access to the second type. Finally, the *modality principle* suggests that pictures should be presented in conjunction with spoken narration rather than on-screen text. Since the visual channel of working memory must process both pictures and text, using spoken narration in place of text can off-load some of this processing burden to the auditory channel (*38*).

Enough Is Enough: Redundancy and Coherence

The *redundancy principle* provides further guidance on using pictures, text, and narration. This principle states that visuals should be combined with spoken narration alone, rather than including text that mirrors the narration (*38*). When both text and narration are present, a learner's attempt to reconcile the incoming sources of verbal information is a cognitive distraction, detracting from the ability to allocate attention to essential processing. Although the redundancy principle runs counter to the notion that providing both narration and text will afford learners the opportunity to choose their preferred modality for verbal information, it has been validated by a number of research studies (*40*). Similarly, the *coherence principle* addresses cases in which adding too much information may actually make material less coherent. For example, research has demonstrated that the addition of extraneous elements such as background music (*49*) or elaborative elements such as mathematical formulas (*50*) may detract from learning. This does not imply that material like formulas—which can be essential to chemistry learning—should always be omitted, but that that the specific goals of instruction for a particular learning resource must be carefully considered and the resource thoughtfully designed.

Breaking Information Down: Pre-Training and Signaling

How can complex information in a multimedia environment be handled to avoid overloading working memory? Several principles have been proposed. As noted above, a learners' prior knowledge has a significant impact on his or her ability to integrate new information; the *pre-training principle* suggests that helping learners to acquire appropriate prior knowledge can ease cognitive load (*41*). For example, before launching a simulation of a somewhat complex phenomenon such as definite proportions, it might make sense to ensure that learners understand the concept of conservation of mass by providing a short tutorial. Another approach to complex material is to utilize signals, or cues, to direct learners' attention to specific elements within the learning materials. This can help the learner by reducing the need to process extraneous material

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(*19*). In an animation about chemical equilibrium, for example, a visual cue might cause different components to "light up" when they are under discussion; in this way the learner's visual search for the pertinent area of the diagram is reduced, leaving more resources available for processing information. Similarly, various types of cues can support the learner in the challenging process of making conceptual connections between corresponding features of multiple representations, such as a rise in temperature of a pictured substance and the rising line on an associated graph. Such cues can be visual (e.g., corresponding colors or labels), spatial (e.g., same relative placement of elements), or temporal (e.g., items appearing simultaneously); connections can also be made explicitly through cues in the narration, and several of these approaches could be used simultaneously (*51*). *Cueing* or *signaling* can include messages that signal learners about the organization of the material itself, for example subject headings or "pointer words" such as *because* (*52*), or can be inherent in the structure of the visualizations provided. To illustrate, one study found that when the same information on time zone differences was presented in two different types of visual charts, students did better on different types of assessment questions depending on which visualization they had used (*53*).

Optimizing the Communication of Information

In any presentation format, designers must make a series of decisions on how to represent information. The processing demands of dynamic representations make these decisions particularly important.

Using Icons To Represent Key Ideas. The Integrated Model of Text and Picture Comprehension (*54*, *55*) draws a distinction between two basic types of representations, or signs: *depictive* and *descriptive*. Depictive representations include pictures, such as photographs or drawings, as well as models or graphs. In general, depictive representations are *icons*, signs that are related to their referents by some type of perceptual similarity—visual or structural features, for example. A descriptive representation, on the other hand, is based on symbols, which are only arbitrarily related to their referent. The word *chair*, for example, represents "a piece of furniture on which we can sit" not because of any similarity between the word itself and an actual piece of furniture, but by convention only. An emerging principle of design for dynamic representations suggests that representing key information in iconic (depictive) rather than symbolic (descriptive) form may be beneficial for learners, particularly those with low prior knowledge of the subject area being taught (*19*, *56*), as well as younger learners (*57*). For example, we found that using icons to represent temperature in our kinetic theory simulation (Figure 5) resulted in higher scores on outcome measures for individuals with lower prior knowledge (*58*). Iconic representations, which by definition relate directly to their referents, require less interpretation than symbolic representations such as text. This means that learners are able to devote more working memory to comprehending the information and constructing their own mental models.

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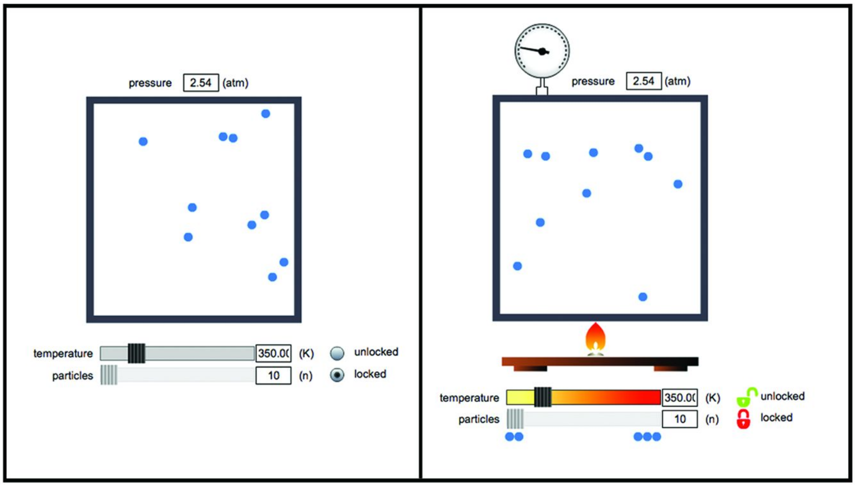

Figure 5. Two versions of the simulation compared the use of symbolic (left) and iconic (right) representations. (see color insert)

The Apprehension and Congruence Principles. Beyond the use of icons, representations should be structured so that the user may readily perceive and understand them, a concept known as the *apprehension principle* (*22*). In particular, this principle suggests that a rigid adherence to strictly realistic depictions may not be the most helpful approach. Many on-line animations of DNA replication depict exquisitely complex shapes moving in real time through a seething mass of colored fluid. However, the rich detail of these representations can be overwhelming to someone seeking to understand the basic principles at work. Sometimes a simplified representation can capture essential information while being easier to understand (*20*). Similarly, the *congruence principle* states that it is more important for a representation to support the desired conceptual model than to conform precisely to reality. For example, a complex process that involves simultaneous events, such as the flow of fluid through a machine, may be represented as a sequential chain of events in order to help the learner comprehend (*20*). In the case of chemistry visualizations, research findings indicate that creating representations which are absolutely chemically correct in every detail can result in materials that are excessively complex and do not support understanding, particularly in novice learners (*59*).

The Emotional Design Principle. Beyond principles related to cognitive aspects of learning, recent research has also shown that affect can impact learning. Studies have shown that positive emotion can enhance a range of cognitive processes (*60–63*). In the context of learning, affect is often considered in terms of motivation (*64*). Moreover, our research has shown that the information design of multimedia learning materials can induce positive emotions in learners that facilitate their comprehension of the material and their ability to transfer their knowledge to novel situations (*65–67*).

Interaction Design

While information design principles address how materials look and how different elements should be combined, *interaction design* involves how the user can control or manipulate materials within the learning environment. Interactivity in a multimedia context involves reciprocal activity between a learner and a learning system; the actions of the learner influence and are influenced by reactions of the system (*68*). Opportunities to interact with visualizations may increase motivation (*69*) as well as the amount of mental effort that a learner invests (*24*), and interactivity is often considered fundamental in supporting a user's understanding of content in a multimedia resource (*27*, *28*). Learning environments can be designed with various types of interactive affordances, and several multimedia principles address this type of design decision.

Learner Control

One particular issue with respect to dynamic visualizations is that because the information displayed can change rapidly, a learner may have difficulty comprehending it in the limited time available (*20*, *27*). According to the *segmentation principle* (*38*), it may be advantageous to have the learner control when to pause or advance the presentation. Discussions of the *interactivity principle* (*20*) and *learner control of pace* (*19*) are similar to segmentation, but somewhat broader in scope, including advanced controls such as rewinding or controlling the speed of the presentation. If learners are able to control the pace of a dynamic presentation, replay segments as needed, and advance to the next segment when ready, they can adjust the allocation of their cognitive resources depending on their own particular needs (*20*); distributing high intrinsic cognitive load over a longer period of time can support better learning outcomes (*19*).

Guidance and Feedback

Teachers often introduce dynamic visualizations, particularly simulations, in order to provide students with active learning experiences that will help them construct rich mental models (*27*). However, many learners do not interact with these materials in a systematic fashion and therefore do not fully utilize the possibilities for learning (*26*, *27*). The *guided-discovery principle* suggests that individuals will learn better in a discovery-based interactive environments if it provides some guidance (*17*, *19*). Guidance can take the form of specific explanations embedded in the learning environment, advice or hints on how to proceed, or assignments that the learner must complete (*17*). Feedback is a specific type of guidance that typically evaluates a learner's responses as right or wrong. Explanatory feedback, which includes an explanation of why the answer was correct or incorrect, has been shown to be particularly effective, especially for novice learners (*19*, *70*).

Reid, Zhang, and Chen (*71*) suggested that guidance for learners in a computer-based scientific discovery learning environment may take three different forms: *interpretative support*, to help activate prior knowledge and guide integration of new information; *experimental support*, to scaffold the process of designing, conduction, and interpreting experiments within the environment; or *reflective support*, to prompt self-awareness, abstraction, and integration of conclusions.

Too Much of a Good Thing: Interactivity and Cognitive Overload

Interactivity is commonly assumed to enhance learning (*68*). However, interactive functions that introduce tasks which the learner must perform—such as moving on-screen elements or advancing from screen to screen—may sometimes impede rather than facilitate learning. Interactions that require a substantial commitment of cognitive resources may leave insufficient capacity for the processing of information; the user's behavioral activity does not always indicate the presence of meaningful cognitive activity. ((*70*); see also (*72*)).

Instructional Tools and Strategies

The provision of guidance is not only a matter of interaction design, but also falls into the category of instructional strategies. In many simulations the learner's task is to explore a virtual environment in order to arrive at conclusions about the conceptual model on which it is based; however, these environments may be difficult for some students to navigate successfully. For example, inexperience in generating and adapting hypotheses, designing in-simulation experiments, and interpreting the data that emerge may impede a learner's ability to carry out systematic explorations, evaluate evidence, and generate an accurate mental model (*26*). To guide and support learners in using such environments, a number of instructional strategies and tools can be incorporated into the design of these resources. *Scaffolding* is a general term that is often used to describe guidance, applying the metaphor of a temporary structure erected to support construction in progress—in this case construction of knowledge (*73*). Based on the work of Vygotsky (*74*), scaffolds are designed to bridge the gap between what students can do by themselves and the learning that is possible with a little instructional assistance (*75*). Vygotsky (*74*) argues that learning depends on appropriately designed instruction, and the metaphor of a scaffold helps us to understand that adult support of student learning is also suitable in the multimedia context. Scaffolding can be gradually removed, or faded, as learners gain expertise.

Starting Simple: Model Progression

The technique of *model progression* provides learners with a simplified model of the environment to begin with; as the learner gains experience the model increases in complexity (*76*). For example, in a study that examined the use of a simulation on the topic of oscillation, participants were given control over only two variables in the first level of the simulation, advancing to five variables in the third and final level tested (*76*). This kind of progression is known as *model elaboration* (*77*). Another approach, *model order progression*, scaffolds learners as they develop an increasingly complex understanding of the relationship between variables, mastering qualitative relationships before specific quantitative relationships such as formulas (*77*).

Guiding Activity: Assignments and Worked Examples

A multimedia environment may contain a large amount of information and may incorporate a number of ways for learners to access, generate, or process that information (*76*). Consequently, it may be challenging for learners to decide what to do or how to go about an investigation. Providing specific assignments or tasks to learners can guide them in selecting appropriate variables, structuring their investigations, and making sense of their results (*76*).

For beginners in a content area, learning to solve domain-related problems can be another challenge. One method of scaffolding this process is to provide novices with a series of *worked examples* (also referred to as worked-out examples), which present step-by-step problems and solutions (*78*). A worked-example resource first introduces the learner is to a principle or concept; illustrates solution steps in one or more worked-out examples, and finally presents additional problems for the learner to solve independently (*79*). To help the learner make the transition between worked examples and to-be-solved problems, steps may be gradually removed, or faded (*79*). Although worked examples are not new in science learning (*80*), using dynamic representations this way affords different approaches to presenting these problems, for example by allowing steps of the solution to appear one at a time. From a cognitive load perspective, learners faced with unfamiliar problems must devote significant cognitive resources to holding a number of items in mind, such as the current state of the problem, the desired end goal, any subgoals, and how to get from the current state to the end goal (*78*). For a novice learner, keeping all these factors in play simultaneously may not leave sufficient cognitive capacity for the development of understanding. Worked examples can lighten this burden. As expertise increases, however, worked examples are no longer an effective approach (*78*).

Strategies To Encourage Reflection

For science learners, engaging in reflection about a phenomenon under investigation may encourage deeper processing and comprehension (*81*). As individuals encounter new information in a dynamic environment, they need to take an active role in making connections between new ideas as well as with their prior knowledge (*38*). Strategies that prompt learners to reflect by making predictions, articulating explanations, and generating alternatives may support the integration process (*82*). Additionally, learners have a knowledge of the experienced world that may be at odds with the way science understands the world (*83*) and reflection can be used to support students to acknowledge such contradictions. With specific reference to science learning, Lijnse suggested that when students arrive in a science class, they already possess a significant fund of conceptual knowledge about the world (*84*). The appropriate approach to science education is not to teach science concepts from the "top down," Lijnse argued, but "to engage with [students] in a 'bottom-up' learning process," in which their own experiential knowledge "guides them in the activity of 'scientificalizing' their world" ((*85*), p. 192).

Multimedia environments offer numerous approaches to prompting these kinds of reflective practices. For example, a simulation about a phase change could provide a text box in which students record their predictions of how quickly an element in a specific periodic group will reach a boiling point, based on its molecular weight compared with other elements from a group they have explored already. Pop-up questions might encourage a user to propose a general principle based on the observations he or she has made. Research has demonstrated that these kinds of strategies can support learning in dynamic environments (*2*, *82*, *86*).

Creating a Context and Motive for Learning

Educators have long acknowledged the importance of basing instruction on what a student already knows and has experienced (*87*). Finding *motive* is also key: Lijnse (*84*) assert that students must be encouraged to *want* to add to their understanding of experience providing students with opportunities to *scientificalize* (*84*) their world through their use of multimedia idealized explanatory models that allow them to address 'why' questions. Equally important, Lijnse asserted, is *problem-posing*: Creating a situation in which a student not only *wants* to learn more, but *sees the point* of learning more through their awareness of the content related reason for their involvement with these simulations (*84*). For these reasons simulations need to have a coherent structure with clear direction and purpose.

Learning Together: Supporting Discourse through Dynamic Representations

The study of chemistry involves molecular processes that cannot be directly observed, making representations critical. Kozma et al. (*11*) suggest that the importance of representations goes beyond their surface features, which can be observed, manipulated, and discussed. A second critical function involves scientific discourse itself. Representations are "inherently social;" scientists rely on them as they collaborate in negotiating and constructing meaning ((*11*), p. 110). Students, too, can use representations in this way. As a group of students collaborate to use a simulation, for example, they may discuss how to approach an experiment or propose alternate interpretations of the data they generate, using representations to communicate to each other. Thus, representations serve a mediating function, becoming a shared artifact between individuals with different viewpoints (*88*). Such artifacts provide students with the opportunity not only to master concepts but to engage in the investigation processes that are typical of authentic science practice (*89*). Dynamic resources can be designed to foster opportunities for investigation and collaboration, for example by providing tools for commenting on each other's work or for creating and managing groups. Because access to available resources can influence the practices of a community, using dynamic representations has the potential to change the nature of classroom discourse (*89*).

Applying Theories and Principles to the Design of Dynamic Resources

How do theoretical and research-driven approaches to multimedia design translate into the development of simulations for chemistry education? The goal of the Molecules and Minds project, conducted from 2005–2013 in the CREATE Lab at NYU with support from the Institute of Education Sciences, was to investigate the implementation of well-designed simulations as a teaching resource in intact chemistry classrooms. Our plan was to develop a sequence of simulations based on theories of multimedia design and best practices in science education, then implement a series of research studies to systematically evaluate a number of specific features of the simulations. By design, these resources would be accessible and useful for a broad range of learners, including individuals from student populations who have historically been challenged in science classrooms.

As a basis from which to explore the impact of multimedia simulations on student learning we selected one of the fundamental chemical theories, kinetic molecular theory, and an associated topic, the behavior of ideal gases. These topics require students to engage in the type of cognitive transitions between observable, explanatory, and symbolic representations needed to demonstrate deep conceptual understanding of chemistry topics and to communicate these understandings. By employing an iterative design process that included development, testing, modification, and retesting, we anticipated that we could add to the base of research on the design and integration of simulations for science learning, developing and implementing a sequence of simulations on the basis of this research. Our goal was to support the communication of key big ideas about the particle model of kinetic molecular theory to a diverse audience of high school students.

Our approach was based on our understanding of models in science learning and our acknowledgment of the importance of supporting science learners in moving between inquiry and explanation. The learning model we developed—the CREATE model of inquiry—emphasizes contextualizing science learning in the everyday; presenting clear and manageable visualizations; supporting active exploration of the simulations; and scaffolding learners as they make connections between the observable, explanatory, and symbolic levels. This understanding of simulations is similar to that proposed by Krajcik, Simmons, and Lunetta, who

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argued that, "appropriate simulations and tutorials can help students learn about the natural world by having them visualize and interact with underlying scientific models that are not readily inferred from first hand observations" ((*90*), p. 148).

Designing Our Simulations: The Importance of Structure

We have discussed the idea that effective instructional materials must incorporate a coherent underlying structure that will support the learner in constructing an accurate mental model (*38*). With this in mind, each of the simulations in the Molecules and Minds project is structured to include the three levels of representation that are critical to understanding and becoming fluent in the field of chemistry: the observable, the explanatory, and the symbolic (*14*). On the *observable* level, a narrative introduces each simulation. This narrative leads into an interactive *explanatory* model, which represents the particulate level. Finally, an interactive graph, on which data appears dynamically as a student manipulates simulation parameters, gives a *symbolic* representation of the relationships between the variables that are the focus of the explanatory model. In the following sections, we discuss each of these levels, including some of the theoretical considerations that informed our design decisions as well as the research we conducted in order to empirically test those decisions.

Presenting the Observable: Using Narrative To Introduce Phenomena

There is no universal principle about where inquiry should begin, but we chose to use narrative as a structure to introduce the observable, or experiential, level. Our goal was that the narrative in each of our simulations would represent an invitation to inquiry, helping learners make connections to everyday life. By utilizing familiar phenomena, we acknowledge that students come to science learning with their own conceptions of the everyday, and that science education is a process in which the teacher seeks to help students understand their preexisting beliefs in the context of formal scientific thinking (*84*). For example, in the Gas Laws simulation we begin with our heroine, Gabriella; her "Everfull" basketball; and the question of why her basketball seems flat in the morning but more inflated in the hot afternoon (Figure 6). The students are invited through the narrative to ask questions and form hypotheses that they can then explore within a specific explanatory model.

Why Narrative?

Research in a number of disciplines supports the use of narrative to introduce scientific phenomena. Studies have demonstrated that expository text, the form commonly used in science textbooks, can be difficult to comprehend because of the lack of text coherence and the demands it places on subject matter knowledge (e.g., (*91*)). Anthropological investigations of narrative also show that consistently, across the world, narratives play an important cultural role and are imbued with purpose and value (*92*). Narratives offer students a tool for understanding that facts are useful for addressing specific questions (*93*), placing students in *science-making* situations rather than the *finished science* situations typical of exposition (*94*).

In contrast to propositions that can be explained, narrative is a form of discourse that cannot be explained but can be *interpreted*. Thus, readers with a broad range of different experiences can make sense of a narrative because its meaning is open to question. Similar to the notion of representations as social objects (*89*), sociocultural studies suggest that narrative provides a structure, a third space, in which people in a community draw on multiple funds of knowledge to make sense of the world (*95*, *96*).

From Descriptive Correlation to Explanatory Models

Our use of narrative as an introductory structure is also a deliberate strategy for moving students beyond descriptive correlations, the form of inquiry they typically experience in school science. For example, in high school chemistry labs, students commonly explore phase change by observing the heating of a solid and its conversion to a liquid. They can record the temperature at which this change occurs, and can learn that this temperature is characteristic for a pure substance. Making connections between the conversion from solid to liquid and the observed changes in temperature is an example of descriptive correlation. However, if we want students to understand these changes, they need to ask *why* questions. *Why* questions associated with this phenomenon requires reference to a molecular model, which our simulation provides. Although descriptive correlations have a place in science, research by Windschitl, Thompson, and Braaten (*97*) indicates that if inquiry requiring descriptive correlations is the only experience pre-service science teachers have of inquiry in science (via the 'scientific method'), they tend not to value or understand the importance of explanatory models to the development of scientific understanding.

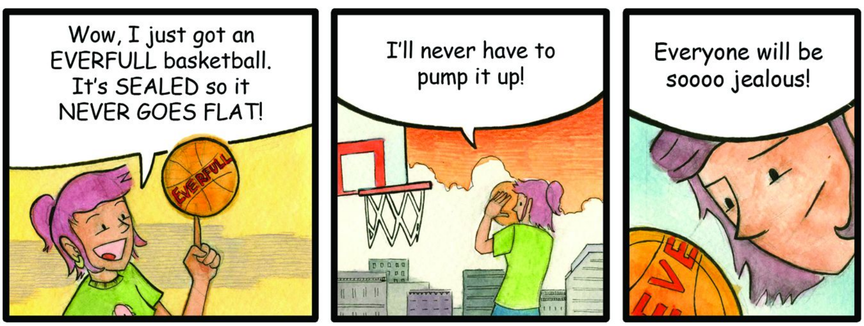

Figure 6. The opening frames of the gas laws simulation narrative introduce Gabriella and her "Everfull" basketball. (see color insert)

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Typically, high school students have even less experience with inquiry than pre-service teachers, and learners may find addressing *why* questions in open-ended model-based inquiry very difficult (*97*). One educational challenge for us has been to establish situations in which students feel the need to explore *why* questions associated with the phenomenon in each narrative, and then to support these students in their explorations.

Developing Narratives for Learning: Applying Theory and Research

In designing the simulations in the Molecules and Minds project, we employed an iterative design model: We developed a prototype for each simulation based on input from high school chemistry teachers as well as curriculum experts; presented the prototype to students and teachers for usability feedback; implemented changes based on usability results; then tested the redesigns in lab and classroom studies. In these studies, we systematically isolated individual factors in order to arrive at a set of features that were empirically shown to enhance the value of the simulations for high-school chemistry learners.

To establish whether the use of narrative was in fact a helpful strategy to support student learning, we compared the performance of students who used the simulation in three different conditions: with an *expository* introduction; a *narrative* introduction; or a *proto-narrative* introduction, which contained narrative elements but lacked a protagonist (*98*). We found that students who viewed the narrative performed better than students in other conditions on measures of recall. Students in both narrative and proto-narrative conditions interacted more with the simulations than did students in the control group. Based on these outcomes, we continued to develop narratives to accompany each simulation.

In follow-up work, we noted a more complex picture of simulation use. An analysis of students' visual attention patterns and log file data of their simulation use revealed a subset of students who possessed sufficient prior knowledge to engage meaningfully with the simulation but demonstrated, on average, significantly less interaction with the simulation and significantly lower learning outcomes (*99*). We wondered whether this could be related to feedback we had received from students in focus group sessions on various narrative scenarios. For example, the popcorn narrative that introduces the diffusion simulation poses the question, "How did Gabriella know that [her brother] had [made] popcorn?" Students discussing the narrative responded with comments such as "that's obvious—it's the smell." We speculated that using a very familiar scenario to contextualize might have an unintended effect: If students think they already know the answer, they may not perceive any need to investigate further. They believe they already understand the phenomenon. With no motive or *need to know*, students do not become engaged in learning (*84*). We decided to challenge students directly through the narrative, a process we called *problematizing*. Rather than simply posing the question, we revised the narrative to encourage students to rethink their assumptions (Figure 7).

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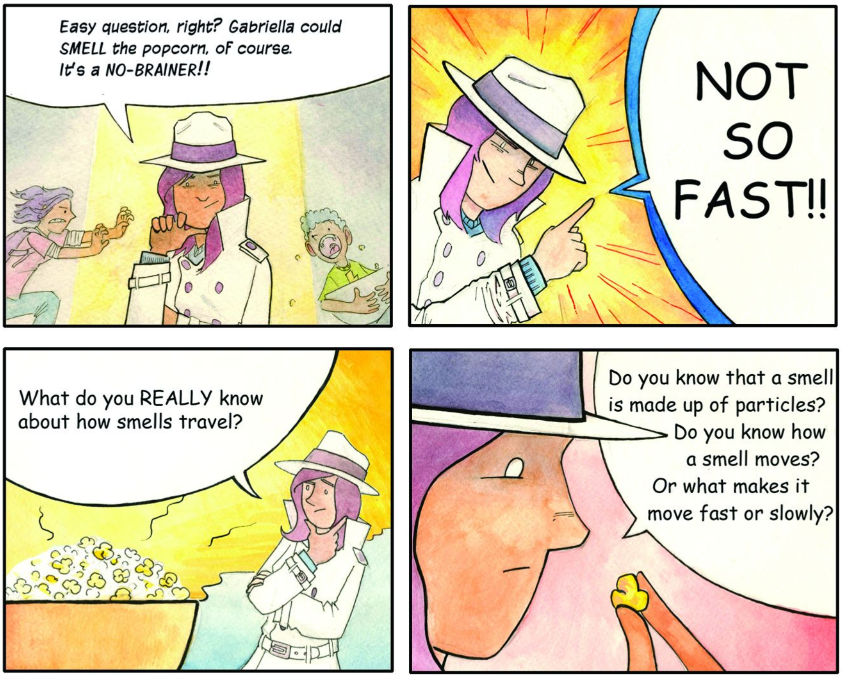

Figure 7. Problematizing narratives can challenge students' assumptions.

When we tested students using the problematizing vs. non-problematizing versions of the narratives, we found that students in the problematizing group had higher scores on the test of transfer. Problematizing also appeared to be particularly helpful for students with low prior knowledge scores: While those in the control group with higher pretest scores also had higher transfer scores, participants in the treatment group had similar transfer scores regardless of pretest scores (*66*). On a qualitative level, students confronted with the problematizing scenario were often visibly startled, then laughed at being taken to task by the cartoon detective.

Presenting the Explanatory: Using a Model To Depict the Particle Level

Earlier, we discussed the idea that effective instructional materials must incorporate a coherent structure to support the learner in constructing an accurate *mental model* (*38*). In science learning, however, *model* has a different meaning. A scientific model is an instrument of investigation that allows us to explore an aspect of nature without observing nature directly. Models represent certain aspects of reality, often simplified or abstracted, and may be language-based (e.g., theories) as well as representationally-based (e.g., diagrams, physical models, and computer-generated images; (*100*)). The challenge associated with developing models for science education is to make them complex enough to include essential elements of the system, but not so complex that details obscure

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the main message on which we want students to focus (*101*). For science learners, the advantage of a model-based inquiry approach is that it situates their questions and hypotheses within a specific explanatory framework. In our simulations, each of the narratives is linked to an explanatory model. The models are abstract, consisting of a representation of a container of moving particles. The user can adjust variables such as temperature, volume, number and type of particles, or pressure by means of sliders or text entries (Figure 8).

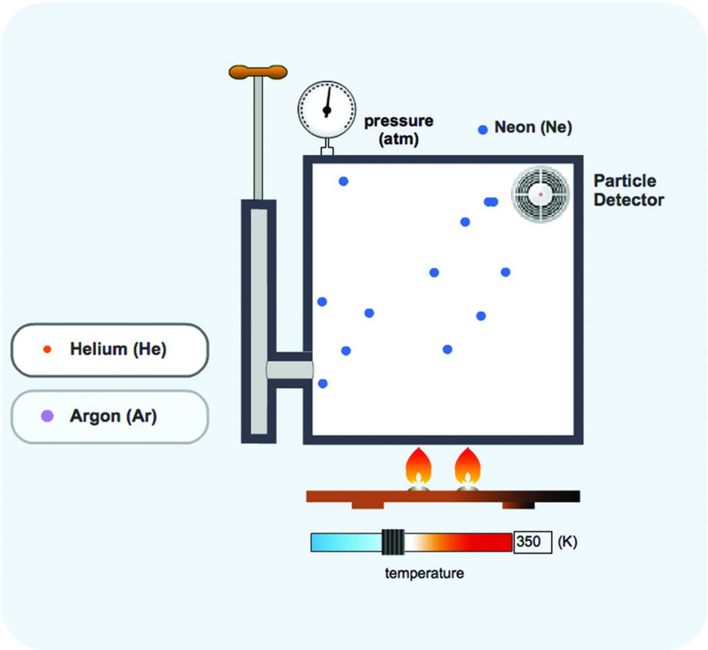

Figure 8. In this explanatory model of diffusion, users can select which gas to inject and adjust temperature using a slider.

The Abstract Conceptual Model and Reality

The particles visualized in our explanatory models behave in a manner consistent with kinetic molecular theory. We want students to use what they learn about a concept from the model to explain another phenomenon—in other words, to be able to transfer knowledge from one context to another. The multimedia experience associated with making models is using a simulation; in structuring this experience we are seeking to support students' developing understanding that they can apply knowledge to a new situation to explain new phenomena. However, the particle model represents a phenomenon that cannot actually be directly observed, and consequently our simulations do not attempt to mimic

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reality. For example, the container is a schematic diagram, not portrayed in three dimensions. There is a school of thought that feels the need to be very literal: If bicycle tires are used to introduce the phenomenon of gases, tires will appear in the explanatory model. However, we have found that such an approach can lead students to fixate on the specific phenomenon—like bicycle tires— rather than on the important explanatory ideas presented in the model, which learners can transfer to another situation.

Idealizations

Our goal has been to develop simulations in which the message—the big ideas—do not get lost in the details of a complex model. We take models as the source of explanations but, as we noted previously, they are also abstractions and simplifications of complex systems that are accepted as part of the natural world. Consider the following:

If x is a gas of a given mass, y, and if all the molecules of x are spherical, possess equal masses and volumes, have negligible size, and exert no forces on one another except during collisions which are perfectly elastic, then if x is trapped in a vessel of variable size and the temperature of y is kept constant, any decrease of the volume of y increases the pressure of y proportionally, and vice versa (*modified from* (*102*)).

This sentence captures the basic principles of Boyle's Law, which students can explore in our simulation of the Ideal Gas Laws. It includes statements about gas molecules such as

- *they are spherical,*
- *they possess equal masses and volumes,*
- *they have negligible size*
- *they exert no forces on one another except during collisions which are perfectly elastic*

These statement are idealizations, and can be typical of explanatory models. Our simulations provide space for both causal and probabilistic explanations, and idealization allows us to limit the variables available for exploration and context.

Applying Principles of Multimedia Design to the Explanatory Model

In designing the look and functionality of the explanatory model, we took into account a number of design principles. For example, labels for each element of the model are located near the feature they describe (spatial contiguity), and the field is not cluttered with extraneous information (coherence principle). We also used the design of the explanatory model as a testing ground for the emerging principle of representing information through icons, and were able to show that the use of iconic representations, such as flames for temperature, rather than symbolic representations, such as the word *temperature*, was especially beneficial for low prior knowledge learners (*58*). Consequently, we implemented the use of icons in all our subsequent designs.

Presenting the Symbolic Level: Designing Dynamic Graphs

In chemistry, the symbolic level provides a convenient script or strategy for summarizing, quantifying, and communicating various chemical properties and processes. Experts in the field of chemistry use symbolic representations with ease, moving naturally across different levels of representation and combining them to communicate their understandings, strategies, and goals (*51*). For example, Kozma describes observations of chemists at work:

> *Representations were everywhere in these laboratories. Structural diagrams and equations were written on flasks and vials filled with compounds. . .They were written on glass hoods and white boards through out [sic] the lab. And they were in notebooks and reference books, and in journal articles and advertisements on bookshelves and bench tops ((51), p. 5).*

While experts have learned to translate effortlessly between these three levels, students often struggle with making the connection between observable, explanatory, and symbolic representations. For this reason, chemistry educators have shown great interest in using animations and/or simulations to assist students in developing a more connected understanding of the levels of representation (*103*). Because the goal of science education is not only to have students learn a body of conceptual information, but to promote the use of those concepts within a context of science as inquiry (*81*), supporting the development of expertise in making these connections is particularly important.

Graphs are a specific type of symbolic representation, which can be useful in displaying data and promoting the observation of patterns in that data (*104*). National science standards (*12*, *105*) stress the importance of using graphs to introduce students to quantitative aspects of chemistry. However, despite the fact that graphs are commonly used in schools for instruction in science as well as areas such as math or social studies, many students are challenged when it comes to using graphs to draw inferences and interpret data (*106*). Part of the problem may be how graphs are presented: One study found that graphs and other scientific visualizations reproduced in high school textbooks are typically accompanied by less guidance than those in either university-level texts or scientific journals (*107*).

Dynamic graphs provide particularly good opportunities to help students make connections between levels of representation, with the potential to help promote "flexible thinking" about the interrelationships between data and graphs and thus support graph comprehension skills (*106*). Linking representations (for example so that the points on a graph change as a learner adjusts the temperature within an explanatory model) may provide an opportunity for students to make "conceptual connections" between them ((*108*), p. 484). Fretz et al. (*109*) speculate that synchronized representations act as a bridge to help students make connections between their understandings and more expert-like techniques. They

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argue further that simultaneous presentation of a model and graph can further support student learning by providing feedback to the student on their use of the model and their expectations or predictions about the relationship between the observable phenomenon and the variables in the model (see (*75*)).

Applying Principles of Multimedia Design to the Symbolic Level

In our simulations, we display a dynamically linked graph side-by-side with the explanatory (particulate) model (see Figure 4). Several multimedia principles contributed to this design decision. Presenting both representations simultaneously, in close proximity, minimizes both *temporal* and *spatial contiguity* problems. We provide *cueing* by using color-coding to help students make connections between variables in the explanatory model and on the graph; clear labeling of the graph provides another cue as to what is being investigated. Learner control of pace ensures that individuals can proceed at a comfortable rate.

Among other research methods, we have investigated how students utilize the simulations by following their visual patterns with eye-tracking technology. The results of one eye-tracking study of our gas laws simulation indicated that students who made more frequent visual transitions between the container or variable controls in the explanatory model and the graph area tended to perform better in tests of learning outcomes (*110*). This raised questions of causality and correlation: Did these students do better because they made more transitions, or were the transitions just a characteristic of students who "got" the material in a different way? To explore this question, we designed *visual scaffolds*, graphic supports that prompt students to make these transitions (Figure 9).

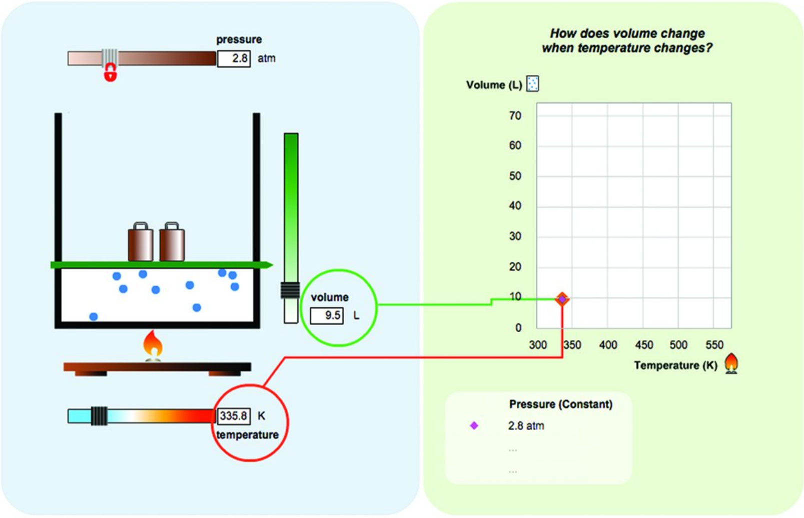

Figure 9. Visual scaffolds prompt users to make transitions between elements in the explanatory model and corresponding elements of the graph.

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In a follow-up study, one group of students received the scaffolds, while another group did not. This study, still in progress, is a good example of how the iterative design process can contribute to the development of theoretically sound and empirically demonstrated principles for multimedia design.

Putting It All Together: Strategies for Exploring the Simulations

In developing these simulations, we were conscious not only of principles that applied to specific representational levels or elements, but to features that affected each simulation as a whole and how students would experience each of those features. Two examples of this kind of consideration were our investigations of *exploration vs. direct instruction* and of *scaffolding*.

Exploration vs. Direct Instruction

In our initial phases of simulation design, we asked whether *free exploration* or *structured investigation* would be most beneficial to learners. In order to explore this issue, we created two versions of our Gas Laws simulation. In one version, students were given a very explicit set of steps to take to explore the simulation. When they clicked each step, they viewed an animation showing the result of the systematic manipulation of the variables of the simulation. In the other version, students were given a set of general goals and instructions and allowed to freely explore the simulation. Our results showed that students in the exploration condition did better in subsequent tests of learning outcomes (*111*). However, in subsequent usability studies of the simulations in intact classrooms rather than our lab, we noted that free exploration did not always provide enough structure, and that students were not getting the maximum benefit from the simulations. This led us to integrate other strategies, such as various kinds of scaffolding, into the simulations.

Scaffolding

As noted above, scaffolding helps bridge the gap between what students can do by themselves and what they can do with instructional assistance (*74*, *75*). In usability studies, we noted several areas of difficulty that seemed to impede learners. We attempted to address these problems through the design of scaffolds that would help elicit prior knowledge, support modeling and questioning, guide exploration of the simulations, and encourage students to draw inferences. As Gobert (*112*) notes, when scaffolding is not provided, the affordances of representations, especially dynamic visual models, may be wasted if students become confused or overwhelmed.

Narrative Scaffolding. We incorporated narratives into each of our simulations to illustrate the observable level, contextualizing the topic under investigation, as previously described. On a broader level, we viewed narrative as a form of scaffolding that could connect the observable, explanatory, and symbolic levels (*113*). Narratives can serve to suggest conceptual links between students' experiential knowledge, based on their daily lives, and the more formal scientific knowledge presented in a simulation (*114*); provide semantic cues, such as questions that capture students' attention at the beginning of inquiry and further assist knowledge comprehension (*115*, *116*); and offer support for connecting complex ideas and events by providing structures and sequences of phenomena under investigation (*117*, *118*).

To achieve these objectives, our narrative scaffolds, presented as on-screen graphic stories, feature a recurring main character. That character is Gabriella, who embodies values of curiosity, questioning, observation, and reasoning through quantification that are central to science. We also have a "detective" character, introduced to frame the concept of inquiry. The detective challenges the learners' assumptions about their everyday experiences, suggests that the simulations will help them understand the phenomenon under investigation, and encourages them to reflect on the connection among the three levels when they have finished using the explanatory model and graph.

Visual Scaffolding. Analyses of verbal protocols in our usability research indicated that learners, at least in the initial stage of simulation use, benefit from explicit links or signals that show relationships between elements within a simulation, for example between the heat of the flames and temperature. In addition to the visual scaffolds currently under investigation to support students in making transitions between elements in the explanatory model and the graph, we implemented graphic changes to provide visual scaffolding. The simple addition of background elements to each screen helps students distinguish elements that pertain to the explanatory level of representation from those that pertain to the symbolic level, while maintaining the close relationship between these two types of representations.

Explanatory Scaffolds. Our research showed that learners often had difficulty in understanding how to structure their investigations of the simulation, as well as in comprehending the relationship between their manipulation of the explanatory model and the information presented in the graphs. In response to these issues, we developed an interactive tutorial scaffold to support learners by scaffolding the difficult concept of exploring three variables. The tutorial walks the learner through the process of selecting two variables to investigate while one is held constant. We also built in features to make explicit the relationship between variables in the particulate representation, such as temperature and pressure, and specific axes of the graph. This tutorial utilizes the principle of pre-teaching, allows learners to control their own pace, and employs scaffolding that fades as a learner achieves competency with the simulation controls.

Implementing Simulations in the Chemistry Classroom

One objective of our simulation development, after the individual simulations and associated lesson plans had been developed, was to test learning efficacy of the full sequence of simulations in intact classrooms. We recruited high school chemistry teachers at public schools in rural Texas and New York City for a two-week effectiveness study. Ultimately we worked with 20 classrooms in Texas and 15 classrooms in New York, providing teachers with the simulations and lesson plans and collecting outcome data on tests of comprehension and transfer as well as process data on classroom use, which includes information such as how much time was spent on the simulations, how the teacher contextualized them, and how students responded. Overall, we found that the simulations helped students with both transfer and comprehension of the content material covered by our lesson plans (for a full analysis see (*2*)). However, as anyone who teaches can testify, a lesson plan is one thing and a lesson can be quite another. Beyond the finding that our sequence of simulations could enhance student learning when integrated into the standard curriculum, our research showed that implementing even the best-designed multimedia resources in a classroom requires a constellation of propitious circumstances—computers that actually work (and have power cords), students who come to class regularly and on time, teachers who investigate the resources thoroughly before using them and are flexible enough to make adjustments as needed, and schools that support teachers by respecting the importance of classroom time. Design factors are critical, yet not sufficient, for the effective integration of dynamic resources in the chemistry classroom.

Moving Forward: Simulations, Animations, and Science-Making

Simulations and animations have the potential to foster a deep understanding of chemistry, including not only facts and concepts, but also an appreciation of the processes and practices of science-making. By allowing students to see what cannot otherwise be seen, to manipulate variables and observe the results of their activity, and to collaborate with others to negotiate meaning and reach conclusions, dynamic representations can change the texture as well as the outcome of classroom interactions. However, developing or choosing these resources—as well as integrating them into the chemistry curriculum—involves a number of critical design decisions.

Over the past several decades, theoretical and empirical investigations of technology for educational use have proposed and validated an array of principles for the design of multimedia resources. In this chapter we have highlighted some of the considerations that are most pertinent to dynamic representations in particular, including principles of *information design*, *interaction design*, and the use of specific *educational strategies*. Because the science of education does not conform to the kinds of laws found in the science of chemistry, it is not possible to establish hard and fast rules about how to design and when to use animations and simulations. Nevertheless, this discussion can lay the groundwork for the kinds of concerns that should be taken into consideration. Individuals who develop animations or simulations for chemistry education, or instructors and curriculum planners who select and implement resources for school use, can use their understanding of these principles to plan or evaluate specific resources.

Research tells us that even the most carefully crafted dynamic resource can differ in efficacy depending on a number of factors: Who are the users? What is the instructional environment? How is use of the resource introduced and guided? Chandler (*35*) observed that "instructors have frequently made the crucial mistake of allowing technology to generate the learning experience rather than using our growing knowledge of cognitive processes to guide us in how we can best utilize technology for instructional purposes (p. 353)." Designing, choosing, and using simulations and animations for chemistry education requires a thoughtful approach that can benefit not only from an focus on content and instructional goals, but an understanding of the needs of individual learners and the process of learning.

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Chapter 4

Linking Animation Design and Usage to Learning Theories and Teaching Methods

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A discussion of several important learning theories: behaviorist, cognitivist, schemata development and dual store memory, and situated learning theories and how these learning theories should inform animations-for-learning design and usage in chemistry is presented. It is argued that learning theories should not only inform teaching methods and assessments, but should also be used to guide the effective development and usage of animations-for-learning. Evidence that animations that have been properly aligned to the operating learning theory and teaching method are more effective than those that are not is discussed. An example of a teaching method that is based on animations that have been aligned to learning theories, and the resulting student performance is presented.

Introduction

This chapter will argue that scaffolding animations-for-learning (from here on, simply: animations) design and usage with learning theories increase the effectiveness of such animation use. Here animation design is taken to include the over-all plan and structure, narrative and content presentation, and the technical and mechanical components (such as choice of buttons, and placement of text). This is distinguished from animation use, which involves both the instructor and student interactions with the animation. It is argued, moreover, that not only should learning theories guide both the design and use of animations, but that the *de facto* learning objectives should do so as well. Here learning theory, the research-based conception of how learning happens within the student, is

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explicitly distinguished from teaching methods, the process that an educator uses to inculcate knowledge. Furthermore, it is implicitly accepted that teaching methods flow out of learning theory, whether the instructor is explicitly or vaguely aware of the learning theory in effect, whether or not the instructor is conscious of using a particular learning theory. As such, if animations design, student use of animations, learning theory, and teaching method all inform each other, there should be an expectation that student performance and student learning outcomes will be enhanced. This chapter will take the stance that learning theory, teaching method, animation design, animation use, learning assessments, and learning outcomes cannot and should not be divorced from each other.

To this end, several learning theories: behaviorist, cognitivist, concept construction or schemata development, and situated learning are presented along with what the teaching methods primarily derived from that particular learning theory might look like. This is then connected to what the teaching method that incorporates animation might look like, and what an animation that was specifically designed for that particular teaching method should look like. Finally, a learning system, named Inductive Concept Construction (IC2), is presented as an example in which animations design and use was guided by specific learning theories and as an example of the kind of teaching method that resulted from an alignment of animations to learning theories. Student performance and outcomes in this learning system are presented.

Towards Effective Design and Usage of Animations

While there are many guidelines, stemming mostly from graphic arts and design (*1*, *2*), for good animation mechanics: high contrast, consistent font usage, color-palettes for the visually-impaired, appropriate image and font sizes, etc., there is research data suggesting that there can be animation design "best-practices" and animation usage. Mayer's research (*3*, *4*) suggests that there are principles in the design of multimedia for the purpose of learning – indicating that the design of animations can be guided by research data. In Mayer's series of experiments, it was shown that lessons are most effectively imparted when information that support each other are presented to the learner by visual and auditory means (Multimedia and Modality principles). Furthermore, learning is enhanced when such auditory and visual information are close together in space and time (Temporal and Spatial Contiguity principles). Narrations should be timed to the visual event, and visual events should occur close together within the computer screen. His research showed that when the visual and auditory channels receive complementary and supportive information rather than the same information (such as printed text that are then read to the user), and that so called "bells-and-whistles" only serve to distract rather than engage the animation user (Redundancy and Coherence principles). Additional research showed that learning is enhanced when hints and guides to information processing is available, when the "next step" in the animation is clear and readily expected, and the learner need not spend valuable mental processing time on dealing with the animation itself rather than its content (Interactivity and Signaling principles). This work clearly indicates that animations and animation designs need not be considered an "art", guided by the "feel" or sensibility of the animator or designer, that there can be some research basis for the choices made in designing any animation.

Mayer interprets the results he obtained from the perspective of a dual store memory model (see later section). He concludes that much of the gains in learning come from reducing the information load on the working memory. My own reading of this is that animations provide ample scaffolding for schemata development (see the next section). Either way, here we see that animation design not only can be guided by research findings, but can also be deeply rooted in pedagogy and learning theory.

Animation use, as opposed to animation design, can also be informed by pedagogy. Assuming that an animation is well designed, that the animations adhere closely to the multimedia learning principles and good animation mechanics, how the animations is used, how it relates within the learner's mind to the lesson objectives, is also important in the overall effectiveness of the animation. An example of a pedagogical concept that applies to animation design and use is scaffolding. Coined by Bruner (*5*, *6*), scaffolding is here defined in the broadest sense as the helpful processes between the educator, learning materials, and learner that allow the latter to pursue meaningful and independent learning efforts. Such scaffolding can be integrated within the animation design as when the interactivity and signaling described in the preceding paragraph on multimedia learning principles is properly incorporated within the animation design. Likewise, scaffolding can be added on by the instructor as when worksheets are provided along with the animation. We've found, for example, that, whether animations are used as stand-alone tools or in conjunction with teacher-centered instruction, it is important that students have a preconceived idea of the narrative of the animation, what they are expected to learn, and what they ought to do when working with the animations (*7*).

Thus we see that learning outcomes from animation based instruction can become enhanced by an understanding of learning theory, both in how these inform animation design, and in how animations become part of the teaching method.

Learning Theories and Resultant Teaching Methods

The Behaviorism Learning Theory defines learning as having occurred if the learner is able to respond to a repeated stimulus with increasing accuracy and celerity (rate of response) (*8–10*). Learning is viewed as the development of specifically targeted behaviors through conditioning. Only the manifested, behavior is relevant in so far as this is measureable; the inner mental life of the learner, generally considered subjective, unquantifiable, and inaccessible, is considered irrelevant. The acquisition of new behaviors by the learner, whether the learners is able to provide a correct response or the correct response at a faster rate, is the objective of a behaviorist and is the central tenet in the Behaviorism Learning Theory.

For a behaviorist –or an instructor who may be unconsciously observing the behaviorist tenets– all relevant planning and organization of learning are external

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to the student, *i.e.* provided by the instructor. The instructor takes on the role of defining the learning objectives, the learning process, and the assessments for the students. Moreover, the focus of the instructor is on improving the accuracy of a student's answer and on teaching methods that develop the student's celerity with those answers. All teaching methods are in support of improving this accuracy and speed. These include: direct instruction – in which the desired responses (and the context in which those responses are desired) are delivered to the learner, memorization and repetition – in which the learner is drilled in the appropriate responses to particular stimuli, and the underlying message that there is a one-to-one correlation between question and answer, such as the number of protons, electrons, and neutrons of any given atom. Assessments in a behaviorist approach include anything that encourages speed (flash cards, timed-multiple choice questions, games that encourage speed and competition at speed) and connecting response to specific questions ("fill-in the blanks", word-matching or word banks, true/false questions). Some of us still remember being shown flash cards with addition or multiplication problems to which the class as a whole would yell out the answer whereupon the teacher would turn the card over and show us the answer. In chemistry, stating the rules of nomenclature and following this with drill-type, in-class exercises, focuses on having the students provide the correct chemical name at speed. Likewise, approaching lessons in dimensional analysis from a numerator-denominator units cancellation emphasizes the correct format of a "one-line" dimensional analysis calculation. These teaching methods were clearly derived from a behaviorism principle of learning.

The Cognitivism Learning Theory rose in response to the behaviorist perspective. It was argued that a behaviorist perspective was severely limited in that much of what is considered learning could not be transferred out of the specific learning environment or context in which the information was obtained. The information on the naming scheme of non-metal/non-metal versus metal/non-metal binary inorganic compounds does not readily transfer to knowing that the bonds in titanium trichloride must have more covalent properties. However, the cognitivists would argue, such knowledge are in fact linked within the minds of "experts". A new learning theory that focused on the inner process, the mental models, the associations that experts make for themselves had to be developed.

The Cognitivism Learning Theory defines learning as having occurred if the learner is able to exhibit "expert procedures" as a product of an inner problem-solving process (*11*). In this context, expert procedures are mental processes that an advanced learner, *e.g.* the teacher, uses in order to solve a problem, and the inner problem-solving process is akin to the models or mental constructs that trained science professionals use as symbolic or mental language in the treatment of a particular concept (*12*). Learning is said to have occurred when a student is able to manifest problem-solving processes that are similar to that used by an advanced learner. When a learner exhibits procedures that can be traced back to a deep, inner mental process, learning is said to have occurred. Thus, in cognitivism, the focus switches from the directly observable and measureable output that are important to a behaviorist to the effort at using the observable behaviors as a window into the inner, thinking processes of the learner. It also switches the focus from a one-to-one correlation between stimulus and response to a general mental process that the learner uses in solving personally generated or personally assumed problems.

This task of using the learner's output as a window into the learner's mental processes becomes difficult when translated to a teaching method. This usually devolves to the instructor wanting to inculcate "proper" thinking processes, getting the learner to think like an expert, and using the learner output as evidence that the learner is able to use such expert and proper processes. Learning, in such a cognitivist perspective, becomes a task of acquiring predetermined thinking procedures –as determined by the expert/teacher– and/or undoing previously learned processes that, in the view of the educator and in reference to the current stage of learner development are considered inadequate. (from Vygotsky's ideas of "Zone of Proximal Development" (*13*) and Piaget's theories on intellectual development (*14*)). While learning is defined as a development within the student, the instructor, functioning as the "expert", much like in the behaviorist model, still plays a central role in identifying the learner's current stage of internal development, and defining the next stages or target progressions. The instructor defines for the student what skills need to be constructed, what concepts need to be developed, and what knowledge associations are most desirable, *i.e.* those of an expert's, those of the instructor. The instructor also defines what learning outputs are acceptable manifestations of the learner's inner process, *i.e.* by defining for the students what are acceptable procedures. Teaching methods include: development of concept maps, construction of expert protocols, and formulation of cognitive associations. These are then assessed by attempting to determine how well correlated the student developed concept maps and concept associations are to what an expert in that discipline would produce. Since the validity of an assessment that purports to establish the level of the learner's inner mental process using the learner's external works or output can be difficult at best, assessments in the cognitive model have given rise to myriad forms of testing, the extent of which goes beyond the scope of this discussion. Suffice to say that the central issue of assessing student output as a gauge of the student's cognitive development is fraught. Consider, for example, the difficulty that a high school teacher with twenty students per section and four sections per day would have in evaluating the completeness of a student-generated concept map on atomic theory, being mindful that, unlike in behaviorist approaches, there is no one-to-one correlation between learning objective and learning output, and that the individual student's output is not the objective but a window into the student's mental process. This would require the teacher to generate a map of what the student is thinking and how effective that thinking process happens to be. The teacher would then be required to follow through and modify or upgrade that thinking pattern, saving the "good" bits, destroying the "bad" and the misconceptions, and encouraging the student to evolve the thinking pattern as a whole. This may work well for instruction on a one-on-one basis, but not generally for a class of twenty, and not for a teacher having three or four such classes per day. As a result, in practice, the translation of the cognitivist theory into a teaching practice or method, becomes an effort in getting the students to use certain "pre-approved" thinking processes, being different from a behaviorist approach in that there is an effort to instill "good thinking processes" instead of good behaviors alone.

Having moved away from the objective and measureable output of the behaviorist, cognitivist theories can be nebulous in practice. Using the learner's output not as an indicator of learning but as an indication of the thinking process that is learning is difficult at best. Cognitivism would crystallize into other theories of learning such as constructivism, schemata development, and dual-store memory models (the latter two will be considered later in this section). However, much as cognitivism was an anti-thesis to the thesis of Behaviorism, and in keeping with a dialectic development of ideas, the synthesis theory, Situated Learning Theory tried to promote the good qualities of the earlier learning theories.

In Situated Learning Theory, learning is viewed as a symbolically mediated activity, a transaction between the learner, the environment, and a specialized community of practice (*15*, *16*). It is symbolically mediated in so far as the learning community has a contextual language of words and images and learning involves this language. It is an activity in so far as learning is viewed as a process entered into by all the participants: educator, learner, the learner's peers, and the learning environment. And since, in this perspective, learning is not centered on the instructor, but in the activity that all participants share and shape, learning is a transaction between the participants. As such, learning in the situated learning model, unlike in behaviorist and cognitivist models, is viewed not as a noun, but as a verb. Learning is not the measureable output of a student nor what is perceived to be happening within the student's mind as a thinking process, but the participant's actions (especially the student's reflective practice) within a specialized or contextual community and environment. It is less about what knowledge the learner accumulates or what information they can retrieve and exhibit, and more about the process that the learner undergoes in order to arrive at the target knowledge. As such, Situated Learning Theory does have an objective component, the observable and measureable activity, that can be directly linked to learning. It also references how this learning as an activity is directly tied to an expert procedure that the community holds, and is linked to the personal and inner life of the learner. Situated Learning Theory, by emphasizing the activity that is learning, has managed to synthesize the qualitative aspects of Behaviorism, and the inner mental life of Cognitivism.

In so far as the practice of Situated Learning Theory is focused on purposeful communal activity, the educator takes a more participatory role in the process. It is the educator's job to understand the process that each individual student is going through and to try and develop an environment that aligns the student's activities with the curriculum or learning standards. Teaching methods that have grown out of an acceptance of situated learning principles include: study-practice-reflection cycles, peer-to-peer interactions (*17*), cooperative learning (*18*), and problem-based learning (*19*, *20*). These methods focus on learning as meaningful activities that allow the learner to be mindful of study as a process. In the study-practice-reflection cycle, the learner is made to recognize the different steps in formulating knowledge: personal and independent study, application of knowledge, and reflection on personal performance and practice outcomes. When done in a cycle, the learner gets to see that learning is not the acquired knowledge but rather the activity itself. Likewise in cooperative learning

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teaching methods, *e.g.* jigsaw method wherein members of a group hold different pieces of information, the learner is made aware that the task of piecing together the different pieces of information can lead to new knowledge. Assessments that lead to metacognition (*21–23*) such as formative and process assessments, evaluations that allow the learner to have a heightened awareness of learning as a process, stem from situate learning concepts. Formal critiquing processes such as that found in Calibrated Peer Review (*24*) (CPR) owe much to situated learning principles. In CPR, a learner's written work is reviewed by different (anonymous) peers and the comments are sent to the learner. The learner then uses this not only to correct his/her own work, but also to calibrate his/her own review of others' work. Learning here is the process.

Schemata Development Learning Theory (*25*, *26*), and the Dual-Store Memory model (*27*), although also focused on learning as a process, both have their roots in cognitivism (*12*). Schemata development speaks of learning as the learner's process by which associations and concept connections (schemata) – hear taken as the mental associations and organized cognitive structures already alluded to in the Cognitivism Learning Theory. The various multi-store memory models speak of how the learner's brain might accept information and store it. In this context, the working memory is where one might temporarily store incoming visual or aural information (*27*). Long term memory, on the other hand, is where one might store processed information for later retrieval and use (*26*). It is very tempting, as I do so here, to link the two theories together and consider that what might be called learning, is the process of transitioning information from working memory to long term memory and that this transition is the conversion of information into knowledge in a schema development process.

Teaching methods that owe their design to Schemata Development Theory and the Dual-Store Memory model emphasize the need to assist the learner in transitioning information into knowledge, to help the learner build appropriate schemata, and to understand the connectivity of such knowledge so that an efficient retrieval process can be developed. For example, since this transition of information to knowledge, from working memory to long term memory, can be inhibited by a Cognitive Overload of the working memory (*4*, *28*, *29*) –a situtation wherein the inherently low capacity of the working memory is overwhelemed with incoming information– teaching methods that have risen from an acceptance of schemata development principles seek to reduce this cognitive overload and allow for processing time. Information is given to the learner in small chunks, the learner is allowed to process the information (into knowledge), before additional information is provided. A simple variant of the 50 min lecture called "lecture bursts" allows for the reduction of cognitive overload. The idea is to deliver concepts in 10 min chunks and intersperse some form of assimilative process such as peer-to-peer discussion, Q&A sessions, or quick application of the just discussed concepts before proceeding to the next 10 min lecture chunk. Likewise, the transition of information to knowledge can be enhanced if the working memory receives supplementary information through the learner's Dual Learning Channels: auditory and visual (*30*, *31*). Teaching method, especially multimedia-mediated information deliveries, emphasize the importance of this dual channels of information reception by supplying supplementary information across the two channels. Teaching methods that emphasize scaffolded guided-inquiry (*32*), multimedia learning (*33–35*), and those that reform traditional teaching methods to allow for ample time for information to knowledge transitions are driven by the schemata development learning principles. These processes can be as simple as requiring students to rewrite their notes into a particular format (a process of developing schemata), or periodically interspersing group activities into the traditional lecture (having the environment and peers calibrate the schemata developed). The objective here is to allow students the time to develop content associations and patterns.

It is important at this point to emphasize that, while the preceding section discussed the relationship of teaching methods to particular learning theories, it is understood that learning is what it is – independent of our attempts to develop learning theories to describe it. While research in learning may develop descriptions of and propose perspectives on what learning truly is, while practicing educators may then design teaching methods based on those learning theories, actual learning may have very little to do with the particular learning theory in operation. Moreover, the effectiveness of a particular teaching method and animation usage may be confounded by the possibility that it could be based on an incomplete learning theory. Believing in a particular learning theory or developing a teaching method based on a particular learning theory may have little to do with what, and to what extent, students actually learn. The importance of learning theory in this discussion then is not so much that it defines for us how a learner might go about the process of developing knowledge, but rather that a belief in a particular learning theory –whether explicit in the mind of the instructor or not– informs the teaching method and assessment that is eventually used.

Also important to research is the possibility that the effectiveness of a teaching method and animation use could be directly controlled by how a particular study defines learning. The operating learning objective, how students perform on an assessment based on those learning objectives, how the assessment is designed to provide evidence of learning as a function of the operating definition of learning, often controls whether a teaching method is shown to be effective. We need to be fully aware of the operating learning theory both in our teaching method and in our assessment.

Linking Animation Design to Learning Theory

The design of any animation reflects the operating learning theory. Whether consciously or as an expression of a subconscious belief in a particular learning principle, the design of an animation, the narrative, what is discussed or omitted, what particular concepts are presented as text as opposed to narrated, the conventions –symbols and patterns– used, all of these point to the underlying learning principles that a designer has.

Certain animations are clearly focused on behaviorist goals. Animations that rely on quick thinking and reflexes as the main mode of engagement, such as a binary inorganic nomenclature arcade game (*36*), are clearly intent on having the students exhibit the ability to make quick and accurate responses to particular stimuli. While it can be argued that there is a naming scheme being applied in a nomenclature arcade game and some thought process is required to make the correct connection between name and chemical formula, this thought process is of secondary importance to the desired outcome: quick and correct responses. Likewise, animations that provide very little interaction – appearing more as animated videos or animated slide shows made to progress by a single forward button –and are heavily focused on providing information, also tacitly subscribe to the principle that learning is about obtaining and storing information, and then retrieving that information – in the relatively pristine form in which that same information was presented – correctly and quickly when needed; an essentially behaviorist teaching practice.

In contrast, certain animations are less interested in correct responses, and are more focused on promoting "correct" thinking in the student. Animations that allow users to develop or construct a conceptual model of a phenomenon subscribe to a cognitivist view of learning. Animations such as those treating the ideal gas law (*37*, *38*) (see also figure 2) in such a way as to allow the learner to investigate the macroscopic phenomena – the relationships of the gas law state functions, and connect these to a particulate conception – what the gas particles are doing in order to result in the observed macroscopic states, while purposely withholding an explicit statement of the conclusions from the students, allow the students to develop a mental model, a conception, of the ideal gas for themselves. This type of animation design is rooted in a cognitivist perspective. When followed with assessments that allow the student to express or exhibit their conceptions, such teaching methods and animations use show a clear acceptance of the cognitivist learning model. In this teaching method, animations and simulations are used to provide an environment in which a learner can develop the good thinking practices, an expert's way of thinking.

Animations that promote the development of mental associations, linking concepts to other ideas, other events, especially when such animations are used in the context of an activity in which the associations students make are made evident not only to the instructor but to the student's peers and the student himself/herself, suggests that the animations designer subscribes to the schemata development learning theory. Such animations, when used in the proper context, can include animations and simulations, animations that introduce case-studies, and animations in conjunction with lab activities. For example, in electronic media supported lab manuals (*39*) wherein a printed text of procedures is coupled to videos of laboratory techniques, animations of chemistry concepts, an animated virtual lab (*40*), and animated report guide, there is some attempt to connect all these different information and processes together and to get the student to make the connections between these tasks. Likewise, in animations that present the same concepts but in different learning domains (macroscopic phenomenon, particulate conception, and symbolic reference) (*41*), again the approach subscribes to the learning principle of schemata development through constructed associations.

Remembering that the Situated Learning Theory focuses on the process as learning, focuses on the transactions made in the learning process rather than on the learning material or content, suggests that animations that are designed to be incorporated into a larger learning strategy wherein learners become focused on learning as a process rather than the content knowledge itself – teaching methods such as cooperative learning (*17*, *24*) or inquiry learning schemes (*18*, *19*) essentially show that the designers are subscribing to situated learning principles. For example, when the ideal gas law animation mentioned previously is used in conjunction with a peer-to-peer discussion and formal reporting (*42*), such a teaching method is implicitly subscribing to a situated learning perspective of learning. In these teaching methods the objective is to make the student's process become evident not only to the teacher but to the student himself/herself. Such teaching practices use animations as a platform for discussion, reflection, and formative evaluation in an effort to make the student aware of learning as a process and for the students to become metacognitive (*21*, *23*, *43*).

The objective of this discussion is not to suggest the primacy of any one particular learning theory, teaching method, animation design or usage. As discussed in the preceding section, it is important to realize that a student's learning is independent of our learning theories. However student learning outcomes are defined by the type of assessments applied, and, as such, are often defined by the operating learning theory. Thus, it is far more important that we, as educators and purveyors of animations, become fully aware of our tendencies and deep-seated learning beliefs as these control what animations we choose, how we use it, how we assess learning based on it, and ultimately, whether our use of animations are effective (as evidenced by our assessments).

The *de facto* learning principle as it is translated to a teaching method is critical to the animations design and effectiveness. An awareness of the potential use of an animation directs the possible animation blueprint choices. Awareness of the alignment of a particular animation to a learning theory directs the instructor to the best use of that particular animation. Awareness of the operating lesson objectives and learning goals directs the instructor on what animations to look for, how those animations should be used, and –if working with an animator– how an animation should be designed. The next section presents a particular example of designing animations as a function of the operating learning theory and lesson goals.

The Inductive Concept Construction (IC2) System as an Example of Effective Animations Usage

Our early efforts in developing animations to support good learning outcomes was initially directed at midsized classrooms of approximately 75 students in the year-long General Chemistry program at the University of Texas-Pan American (*39*, *44–47*). Students in this program had abysmal dropout and failure rates ranging, depending on instructors and standards, from 30 to 80%. Data from the school years (SY's) 1997 and 1998 showed a dropout and failure rate of 36% when using a traditional lecture and textbook teaching method and focusing on algorithm and memorization type assessments. Augmenting the traditional teaching method with technology tools such as PowerPoint (.ppt) lecture notes and online course tools such as Blackboard (then WebCT) had little impact on the dropout and failure rates, which in 1999 and 2000 held steady at 36%

despite the technology infusion from .ppt and WebCT. The percent of students with A's did increase from 15 to 26%, showing that such low-level technology augmentation can have an impact on the top-tier students. However, these courses had traditional assessments that were memorization and protocol or algorithm-based. Taking from the seminal work of Nurrenbern and Pickering (*48*) and the follow up by Sawrey (*49*), we decided to incorporate conceptual questions in our General Chemistry assessments. In 2001 and 2002, the assessments were modified to include 30% worth of concept-based questions – the dropout and failure rates increased to 47%. Thinking that the concept-based questions were not properly supported by a concept-focused teaching method, the whole course was revamped in 2003 and 2004, the .ppt slides were reworked to focus on concepts rather than algorithms, and the quizzes leading up to the exams were changed to ask essay-type questions focused on conceptual understanding. The intent was to send the message to the students that the focus of the course was on conceptual understanding and not algorithmic problem-solving. The percentage of conceptual questions was also increased to 60%. The dropout and failure rates increased to 81%. It appeared that traditional lecture and textbook approaches, even when infused with low-level technology such as .ppt slides and online course tools (WebCT), and ostensibly modified to be more concept focused, could not prepare students to think conceptually in General Chemistry. A different teaching method seemed to be required, and, perhaps, a teaching method that was based on a different principle then from where direct instruction, lectures, and textbooks were founded.

In 2005 and 2006 we published a few articles suggesting that animations could support conceptual thinking in the General Chemistry program (*39*, *44*, *45*). We showed that students using animations did better on conceptual questions than those who received .ppt notes –even when the .ppt slides were replete with transitions to simulate animation. Students in the flash and .ppt groups performed equally well on information retention and algorithm/exercise type questions, but students in the flash groups performed much better than their .ppt counter parts on concept questions – indicating that animations had its strongest effect in allowing students to develop schemata, in promoting the development of cognitive associations and structures. In a similar study, the lab manual of an essentially verification-style (as opposed to an inquiry style) lab was changed so that instructions and pre-lab instructions were replaced with concept-focused animations and videos of techniques, and the printed manual was paired down to include only process guides (with space for students to write in the actual steps that they planned to do) instead of the then standard step-wise instruction or "cookbook" lab manuals (*39*). This produced markedly higher overall grades and fewer dropouts and failures from the animation-supported cohort. Again, this seemed to indicate that if the goal is to improve conceptual understanding (as evidenced by concept tests and the ability to perform concept intensive processes) then an overhaul of traditional teaching methods is needed. Moreover, one way to do this is to incorporate concept focused animations. Simply refocusing traditional teaching methods to a more conceptual approach did not seem to have as strong an effect as developing a teaching approach from a learning theory that is particularly focused on conceptual understanding.

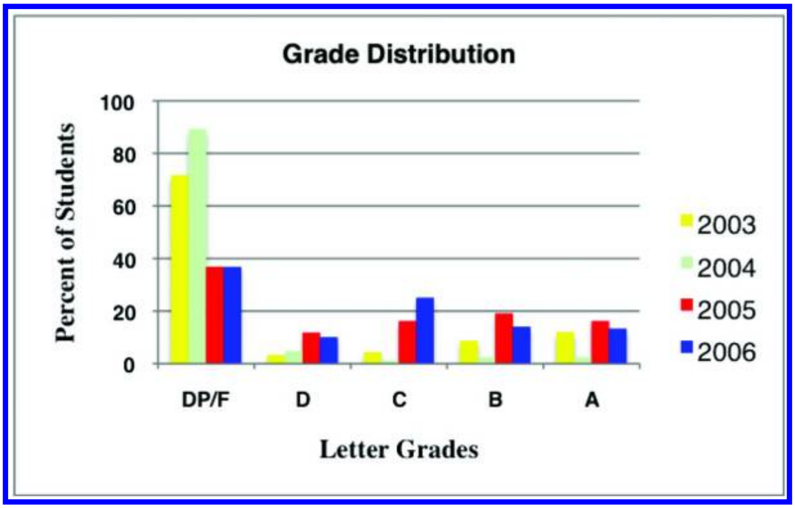

Figure 1. Percent of students receiving particular letter grades in 2003-2006.

In 2010 we published a series of studies that showed that lectures and textbooks could ably be replaced by concept-focused animations and students (studying general science at grades 3-5 and chemistry in high school, as well as college level) receiving this alternative approach to teaching performed equally well or better on standardized tests (*50*, *51*). Finally, in 2011, we published the completed study started in 1997 and showed that students who received a radically different teaching method that incorporated animations, peer-to-peer discussion, and formal reporting procedure – no lectures and no printed textbooks, even when given assessments 60% of which were concept questions, performed much better than those who received technology-infused traditional lectures and textbooks (*47*). Part of the data reported is shown in figure 1 (the light colored bars are for the “baseline” years, with the darker bars for the novel implementation years). The drop-out and failure rate for the three implementation SY’s of 2005 – 2007 was an average of 37% for students receiving this novel learning system and an assessment in which 60% of the questions were concept-based, dubbed Inductive Concept Construction (IC2, meant to sound like: “I see too”) – a remarkable difference compared to the 2003 and 2004 SY’s failure and drop-out rate of 81% – in which concept-focused lectures, .ppt slides, and online course tools support was provided, with assessments in which 60% of the questions were concept-based. It is important to note here that over the course of this study the SAT and ACT scores of students entering the General Chemistry program at UTPA had a slight downward trend (for example, the science ACT of students went from 18.2 in 2002 to 17.7 in 2006 in a steady downward trend). The determining factor for such a radical swing in performance scores seemed to be the equally radical change in teaching method.

The IC2 learning system relied on a foundation of animations that were specifically aligned with the *de facto* lesson objectives. In designing each animation module, we first reflected on what was the primary objective in a

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particular lesson – making no judgement on the value of that objective but accepting what it is that how treated and tested were strong indicators of what we were actually teaching and wanting the students to exhibit. This was a particularly difficult step since we were predisposed to want our lessons to be all conceptual and cognitivist (wanting, as it were, to be higher up on Bloom's Taxonomy). However, if, for example, all we did in stoichiometry was teach the dimensional analysis method of solving word problems that required the prediction of masses and moles, then we had to admit that we were not touching the conceptual aspects of stoichiometry, and if so, then our animations should focus on having students mimic exactly a protocol that we would teach them (essentially a behaviorist objective or a very basic "expert" process). On the other hand, if, for example, we wanted students to intuit that the lessons of stoichiometry applies to pictures of objects (no masses), or transfer the knowledge of stoichiometry to understanding why lithium hydroxide and not sodium hydroxide is used as carbon dioxide scrubbers in planes and spacecrafts, then we had to take a more cognitivist approach. We then looked at what teaching methods would best apply the operating learning theory used. Only then did we think of how best to structure animations that would serve those lesson objectives, learning principles, and teaching methods.

For example, when, in the case of learning the nomenclature rules for naming binary inorganic compounds, our objectives were clearly behavioristic; the correct chemical formula was required –at speed– when given the chemical name or vice-versa. We intended to use teaching methods that were focused on direct instruction and drills. As such, two animations were developed. The first module would provide students with all the rules, show how these rules were used, and give students exercises as practice. This animation was little more than a set of static slides with narration and a few "animated" pointers and buttons. The second animation was the "chemHopper" game (*36*) (a screen shot is shown in figure 2a) focused on creating a fun, drilling exercise in which a student, using the keyboard, controlled a robot and made the robot "hop" from platform to platform. In this game, the only "safe" platforms were those that contained chemical formulas that had a corresponding chemical name in the four tumblers at the bottom of the screen. By having the platforms sit on a treadmill that scrolled to the left of the screen where an "electric field" (the emitter is shown in the figure under the "level 02" text) would destroy the robot if it got pushed there by the treadmill, speed in accurate decision-making was encouraged. At higher levels, the treadmill would scroll faster, erroneous chemical formulas would be included, assorted "power ups" (the ability to clear a platform with a "laser" tool, for example), and speed trials were provided to increase engagement and behavioristic thinking speed. It was determined, for example, that in the chemHopper game, if a student could score higher than a certain number of points, that student would invariably get 100% correct on the nomenclature section of the summative examinations. Students in later trials were told what the target score in the game was and those students who persevered to this score always got 100% correct on the nomenclature questions. Note that, since we were taking a behaviorist perspective on learning, it was not important to know how the students got to the answer, or what inner mental processes a student was going through in order to get to the answer, the only learning objective was to have the students answer questions with accuracy and celerity.

Figure 2. Screen captures of animations used in the IC2 learning system (a) when the lesson objective was behavioristic, and (b) when the lesson objective was cognitivist, concept construction, and/or schemata development.

In contrast, when building conceptual constructs, schemata, was the lesson objective, animations that focused on allowing the student to make mental associations were developed. In such cases, the focus switched from the behavioristic direct instruction and drills to allowing students to build the concepts for themselves. This meant that animations and teaching methods had to be designed that *did not tell* the students the target lesson. Rather, the students, through the use of the animations, discussion with their peers, calibration of knowledge through peer critique, steadily constructed the knowledge for themselves (schemata development and situated learning). For example, in the treatment of gas behavior and ideal gas (*37*) (screen capture of the animation is shown in figure 2b), the students could use the animation to investigate the relationships between internal and external pressure, volume, amount of gas, and internal and external temperatures. At no point were the students informed of what the “correct” conclusions were. There was no mention of Avogadro’s, Charles’, or Boyle’s Law – these terms were added only at the culmination of the lesson when the knowledge was already established and required “labeling”. Students were also expected to derive for themselves the more difficult particulate conception or statistical mechanics explanation of the macroscopic phenomena. Checks of the “correctness” of their conclusions were provided through peer-to-peer cooperative learning, inter-group critiques, and formative in-class reports (also peer-critiqued).

Since the animation was designed to be studied out of the classroom setting, we were very careful to follow Mayer’s multimedia principles (*3*, *4*). Narration that was timed to the action on the screen was provided (in keeping with the multimedia and temporal contiguity principle, and the dual learning channel theory). Since UTPA is a state school, any multimedia provided had to allow for the Americans with Disabilities Act and concessions against good animation design principles had to be made and a close-captioning system (point 1 in the figure 2b) was incorporated even if this went against the Redundancy Principle. This captioning system was off by default to minimize issues with spatial contiguity. The narration was carefully timed so that when animations like indicator arrows appearing on screen (point 2, fig. 2b) and became the visual focal point, this was also the focal point of the narration. The viewer could control the pace of the concept construction using typical onscreen video-play back buttons (point 3). After a description and preliminary investigation of the components, the learner could then manipulate the onscreen objects such as the gas pump (point 4), the thermal jacket (point 5), the piston clip, which could either keep the piston in place (holding the volume steady) or, when removed, would allow the piston to move up and down freely (point 6). Several indicators such as a thermometer and internal and external pressure gauges gave feedback on the status of the macroscopic system that could then be related (when the concept development moved to this part of the lesson) to the particulate conception of gas particle motion resulting in the macroscopic behavior (point 9). A guide as to what the viewer ought to investigate was provided onscreen (point 7). The idea behind such animations then was to provide students with sufficient background information (it has been shown that the failure of some inquiry processes stem from not having sufficient background information (*32*, *52*)), guidance as to what mental constructs and associations might be appropriate to build, and an environment where a student could safely (no sever penalties) and effectively inquire.

Since a cognitive, concept construction, and/or schemata development approach to learning required the instructor and student to become aware of the inner mental process that a student goes through in the treatment of the lesson, students were required to go through the concept development animations and then report out their knowledge to the class. This was done in several ways: classroom time was devoted to students verbally reporting their knowledge, having students critique each other's knowledge report, the instructor correcting any misconceptions (done immediately in order to reduce the propagation and entrenchment of bad ideas), and regular quizzes that were focused on allowing the students to show their concept structures (essays, drawings of particle activity, etc.). Thus, the learning cycle in the IC2 learning system included: students individually going through the animations, online quizzes prior to the class period in which students were encouraged to answer as a group – promoting peer-to-peer discussion prior to the class period, knowledge reports (either as a group or as individuals) in class, student critiques of others' knowledge reports, instructor-centered misconception corrections, formative and summative quizzes. This cycle was done for each lesson or unit that was considered to have an operating cognitivist learning principle.

Emphasizing the need for students to understand that learning is a process (as dictated by the Situated Learning Theory), the program took the individual animation-based learning into a cooperative, peer-to-peer learning process wherein the students' conceptions and misconceptions could be tested and revised by discussion among peers – either within the group or during the formal reporting processes. It is important to emphasize that in this learning system, there are no direct instructions, no lectures, and all that is done in class are the reports, critiques, misconception corrections, and formative and summative assessments. It is also important to note that the knowledge reports and student critiques were set in formal patterns. Reports of concepts were required to come in the form of: a thesis statement, expansion of the thesis statement, and exemplification of the thesis statement. Reports of algorithmic analysis processes came in the form of reporting the essential algorithm process followed by the application of that algorithm. Either a mathematical equation and algebraic process was reported with the numbers manipulation being of least importance, or the analysis strategy was reported first, followed by the implementation of the strategy. A complete student report critique involved the following steps: restatement of the critiqued student's report, statement of any misconceptions and/or incomplete ideas, and a statement of how the critiquing student would have reported the knowledge. While the reporting and critiquing schemes allowed the instructor and the students to become aware of the students' knowledge constructs, making the process formal allowed the topics to be covered with some speed – so that the entire ten or so chapters per semester could be covered with some meaning and depth.

We believe that this is a clear example of proper alignment of animations to *de facto* learning objectives, of the use of animations in a classroom setting that subscribed to both Cogntivism and Situated Learning theories, and of such a process that allowed for student performance outcomes well above traditional teaching methods. It seems clear that well-designed animations with clear learning objectives coupled to teaching methods that subscribe to the most modern learning theories can result in highly positive student learning outcomes.

A Possible Future for Animations and Learning

As we look to the future to see the place animations may have in the learning of chemistry, we cannot help but look to the growing discipline dubbed: New Literacies. This study of the new modes and ethos of discourse being actively defined by the digital native and resulting primarily from new technologies and electronic media offers learners multimodal, semiotic resources for the representation and communication of ideas (*53–56*). Data from New Literacies research indicate that the new, socially constructed modes of producing and presenting meaning are highly engaging for students, highly collaborative, and occurring in affinity spaces where play, popular media, and traditional as well as informal learning may intersect. Leveraging New Literacies practices into the goals of science learning may result in positive gains not only in science knowledge but also in attitudes toward science and learning – even as learning itself is being redefined for and by the digital native.

We have already seen that well-designed animations, guided by the principles of multimedia learning, and scaffolded by both the expected student use and the true learning and lesson objectives can have very highly positive impact as evidenced by student performance. This is even more so when the animations are used in teaching practices that are derived from an understanding of Situated

Learning Theory. We can only expect to get better at preparing animations and developing appropriate animations usage as we improve our understanding of the place of animations in science learning.

In this future in which new technologies, e-media, modes of discourse are seamlessly and organically integrated, traditional teaching methods of lectures and printed textbooks have diminishing effectiveness. We expect that animations, highly interactive e-Books, and student-centered inquiry-based learning will become even more highly relevant, and learning as described by the theories from Situated Learning will guide teaching method and practices even more than it does today.

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Chapter 5

Insights from Using PhET's Design Principles for Interactive Chemistry Simulations

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Since its inception in 2002, the PhET Interactive Simulations project at the University of Colorado Boulder has developed over 125 interactive simulations to advance science education. In addition to the goal of promoting student conceptual understanding of science, PhET simulations aim to engage students in scientific exploration and to increase student interest in science. PhET simulations are thus designed to be fun and interactive, to connect to the real world, to provide multiple representations, and to allow rapid inquiry cycles. The PhET project is guided by cognitive research on how people learn, discipline-based research on student conceptual understanding, and research on the design of educational tools. We also test each simulation using student interviews and study the use of simulations in a variety of educational settings. Based on this experience, we have developed a set of principles for creating simulations that encourage investigation and sense making. In Part I of this chapter, we introduce our theoretical perspective, project goals, and describe our design principles and process – focusing on their application to interactive chemistry simulations. In Part II, we highlight a number of simulation design challenges specific to chemistry, drawing insights from student interview results.

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Introduction

An extensive body of research has demonstrated that computer-based animations and simulations can increase student conceptual understanding of chemistry (*1–5*). Several studies have shown that animations can be effective for enabling students to develop mental models of chemical processes at the molecular level (*6–11*). Other studies have shown that animations can help students develop an integrative understanding of chemical phenomena across macroscopic, particulate, and symbolic representations (*12*, *13*). While a comprehensive base of published research on simulations for chemistry is still forthcoming, there is agreement that interactive simulations offer great potential for supporting student learning (*14*, *15*).

The PhET Interactive Simulations project focuses on understanding and leveraging the potential for improving science education with interactive simulations through research and development. Since 2002, the PhET project has developed over 125 interactive simulations (sims) in support of this mission. PhET sims are designed to be dynamic and highly interactive, to make the invisible visible, to scaffold inquiry by what is displayed and what is controlled, to provide multiple representations, to encourage multiple trials and rapid inquiry cycles, and to provide students with a safe environment in which to explore scientific ideas. In addition, PhET sims are designed to make learning engaging and fun. PhET sims are readily disseminated and incorporated into classrooms: they are easily and freely distributed over the web (http://phet.colorado.edu), and they are designed to allow for flexible use that addresses a variety of learning goals and integrates with diverse pedagogical approaches.

We use one of our newest chemistry sims to illustrate the PhET design philosophy. The *Beer's Law Lab* (Figure 1) sim was designed to enable students to examine how concentration affects the absorption of light. *Beer's Law Lab* uses tabs to scaffold student inquiry and to support construction of conceptual understanding. In the "Concentration" tab, students can explore multiple ways to change solution concentration. They can shake solute into the beaker and add water from a faucet, and they can perform actions not possible in the real world, such as rapidly evaporating water on command. Students can also measure the concentration and consider why the concentration value is constant when they remove solution or after they saturate the solution.

The "Beer's Law" tab was designed to enable students to discover the relationships between concentration, path length, and absorbance. Students can click on the red button to turn on the laser and observe how the light is absorbed by the solution. They can use a slider to change the concentration or drag the yellow arrow to change the path length, and observe the effect on absorbance. To investigate absorbance relationships quantitatively, students can enter a value into the concentration textbox and use the ruler to measure the path length. Students can also use the drop-down menu to compare solutions of different solutes. If the "fixed" radio button is selected, the laser defaults to the wavelength of maximum absorbance for that solute. If the "variable" radio button is selected, students can use a slider to change the wavelength and observe the effect on absorbance.

Because the dynamic and interactive nature of PhET sims is hard to convey in writing, we encourage the reader to explore some of the sims before proceeding.

The goal of this chapter is to present the theory and experience that informs the design of each PhET chemistry sim. In Part I, we describe the learning theory and research that underlies PhET sims, the broad goals that guide PhET sim designs, and the research-based PhET sim design principles. This discussion expands upon prior work (*16*) and focuses on the application to chemistry sims. The process of applying our design principles to the creation of chemistry sims revealed several challenges specific to chemistry. In Part II, we describe these challenges and provide design approaches we have used to address the challenges. Throughout the chapter, we draw examples and supporting evidence from our extensive collection of interview data.

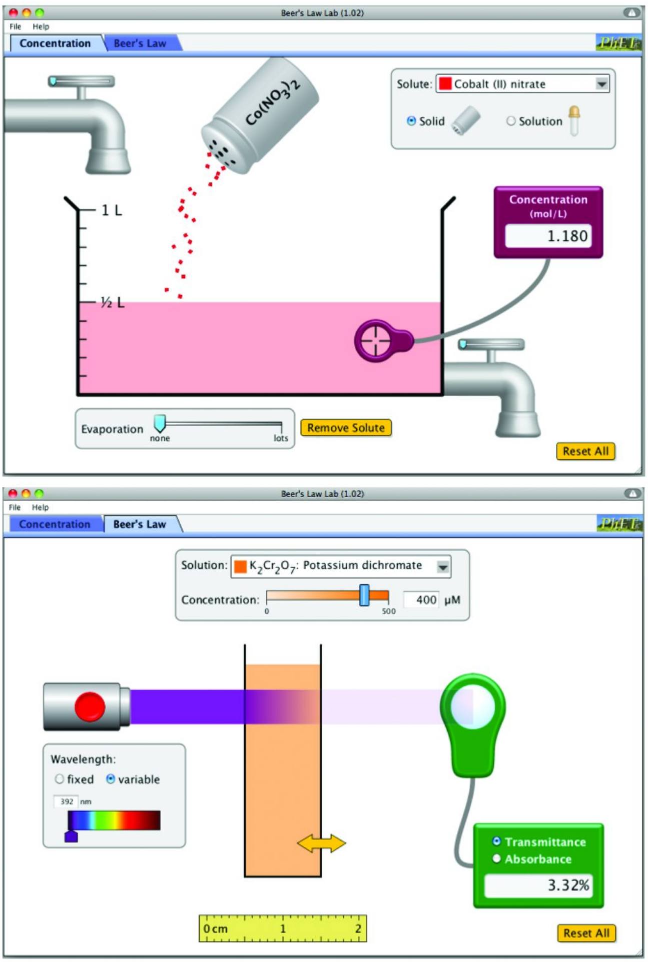

Figure 1. Snapshots of the Beer's Law Lab sim, including the "Concentration" tab (upper) and "Beer's Law" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder. (see color insert)

Part I: Theory, Goals, and Principles

Theory and Research Base

The PhET design philosophy is rooted in the theoretical perspective that understanding is constructed by actively engaging with content (*17*). Ideas are formed and refined based on observation and feedback from experience. Consistent with this view, we design sims to encourage and support the active process of *constructing* knowledge, an interactive exchange between the student and the content, rather than using sims to *transmit* knowledge. Tools – including books, diagrams, lab equipment, calculators, videos, computer programming languages and sims – can play an active role in learning by mediating the learner's engagement with the content (*18*). Each tool has characteristics which influence how students engage with the content. Sims are tools with unique capabilities. These capabilities can be harnessed to frame student interaction with content in productive ways that are informed by what is known about learning. We also attend to the idea that prior knowledge, experiences, and cultural norms influence and shape our learning experiences. We seek to help students build from prior knowledge they bring to the sim learning experience and knowledge they gain within the sim environment itself.

Our perspective is further influenced by research findings from cognitive science and education research (*19–21*). Research on expertise has shown that development of expert competence requires acquisition of factual knowledge and development of an organizational structure that allows for efficient retrieval and application of ideas (*22*). In addition, experts monitor and reflect on their own understanding, a skill required to become self-directed learners (*23*).

Our sim design principles include explicit efforts to support development of both the knowledge structure and learning habits of experts. Feedback, for instance, is a critical component that aids learners in forming mental models and organizational structures, and provides cues to refine their understanding.

Other influential research includes findings that motivation and perspective towards learning significantly impacts learning choices, approaches, and outcomes (*24*). The sim designs frame the learning activity around sense making and growth of understanding, as opposed to knowledge demonstration and answer making. In other words, the experience is more about learning than knowing. Excessive loads on working memory can prevent learners from effectively processing information (*25*). Through the design of sim features we can reduce extraneous cognitive load and direct cognitive attention.

Finally, we draw from sociocultural perspectives and recognize the critical role of context in learning (*26–29*). While sims provide students with new possibilities for engaging with science content, the nature and effectiveness of the learning depends not only on the design of the sim, but also the details of with whom and where it is used, how it is integrated into instruction, and under what conditions. Understanding how these contextual factors influence learning with sims is an important area of our research. In this chapter, we focus on the tool itself and show that well-designed sims can support knowledge construction in a uniquely engaging and effective way.

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Design Goals

Our sim designs are influenced by pedagogical and accessibility goals (Figure 2). The pedagogical goals are based on and aligned with our theoretical perspective on learning. While each sim design is influenced by content-specific learning goals, we have developed a set of goals for students, which are broadly applicable across science topics. The pedagogical goals include science process and affective goals as well as content learning goals. Many of the goals – such as actively engaging in scientific exploration (*30*) and developing expert visual models – align with national science standards (*31*) and constructivist perspectives on learning (*17*). The goals influence the choices made during the design of each PhET sim. Our accessibility goals also drive broad design decisions.

Pedagogical Goals

PhET Interactive Simulations will support students to:

- **Engage in scientific exploration.** Students will pose their own questions, design experiments, make predictions, and use evidence to support their ideas. Students will build on their prior knowledge, monitoring and reflecting on their understanding as they explore.
- **Take ownership of the learning experience.** Students will perceive a sense of autonomy where they can direct their own exploration of the sim.
- **Develop conceptual understanding.** Students will develop an understanding of expert models. Students will deduce cause-effect relationships and coordinate across multiple representations.
- **Make connections to everyday life.** Students will connect formal science ideas to their everyday life experiences and recognize science as a tool for understanding the world.
- **View science as accessible and enjoyable.** Students will engage in authentic science practices and develop their identity as a person who uses scientific reasoning. Students will demonstrate further interest in science.

Accessibility Goals

PhET Interactive Simulations:

- **Are freely accessible to everyone**. All sims are freely available from our website. The sims can be run online or downloaded individually for offline use and redistribution. In addition, the entire website can be downloaded and installed on an unlimited number of computers.
- **Enable use across diverse educational environments.** PhET sim designs create an open environment that provides teachers with flexibility on how to integrate the sims into instruction. PhET sim designs enable use in lab, in lecture, at home, in virtual schools, in informal education, and support a range of pedagogical approaches.
- **Maximize usage by minimizing barriers.** Our choice to adopt a Creative Commons attribution license has resulted in integration of the sims into commercial materials, allowing the sims to reach more teachers and students. We also support translation of the sims, allowing volunteer translators to bring the sims to students in their native language.

Figure 2. Pedagogical and Accessibility Goals. Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

The evolving technology landscape – the emergence of tablets, for instance – requires ongoing evolution of our design choices to support these goals. With over 100 million sim uses since 2002, our efforts to achieve broad dissemination and accessibility have shown evidence of success.

Design Principles

The PhET project has developed a set of principles that guide the design of each sim. Both the principles and the design approaches we use in applying these principles are informed by our own research and design experiences as well as research from education technology, design, and science education communities (*32–37*). New challenges – such as applying the design principles to new disciplines – have provided opportunities to advance our understanding of sim design and our collection of effective design approaches.

Implicit scaffolding through sim design has emerged as a particularly powerful approach – one that enables sims to simultaneously support achievement of process, content, and affective goals. Implicit scaffolding aims to retain a student's sense of autonomy while creating an environment in which multiple investigative pathways lead toward the desired learning experience. Successful designs leverage what students know (e.g. faucets supply water), cue important factors through intuitive designs (e.g. cuing attention to key parameters to investigate by using sliders), tap into natural curiosities (e.g. spark "what if?" questions), and support building of knowledge (e.g. using tabs to scaffold complexity). When effective, the implicit scaffolding allows students to perceive the sims as engaging, open exploration spaces – while simultaneously providing the cuing to guide students to productive interactions with the sim.

Achieving effective implicit scaffolding is a design challenge. Careful design of perceptible affordances and productive constraints into sims has been particularly useful for addressing this challenge (*33*). *Perceptible affordances* are what a user of a tool perceives as a possible and productive action with that tool. For instance, we use faucets with sliders in many of our sims. In this way, users readily perceive that these controls are ways of adjusting parameters in the sim, are readily able to make these adjustments, and can observe the results. *Productive constraints* restrict the actions that a user can take and, like affordances, can be purposefully built into sims. Productive constraints are important for implicitly guiding the use of a sim; productive constraints can restrict the user from taking unproductive actions while encouraging productive actions. For instance, in the "Concentration" tab of the *Beer's Law Lab* sim (Figure 1), students are not able to add more water when the container is full. This productive constraint removes the possibility of students being distracted from the learning goals by overflowing the container, and suggests to students that exploring water volume from 'full' to 'empty' may be useful. In interviews, we have observed students adding water to the container until full, then either exploring other ways to change the water volume (evaporating or draining) or moving on to other productive explorations, such as changing solute type. Productive constraints keep users within a parameter space of the sim that is productive for learning.

Other design approaches also help achieve effective implicit scaffolding. We pay significant attention to: the context used to present the topic – e.g. shaking salt or dropping dye into water, the choice and placement of controls, and the design of visual representations and feedback. Ease-of-use is critical for implicit scaffolding to be effective, so we also prioritize designing an intuitive interface. We describe our current design principles below, detailing approaches used to apply these principles to chemistry sims and drawing specific examples from the *States of Matter* (Figure 3) sim.

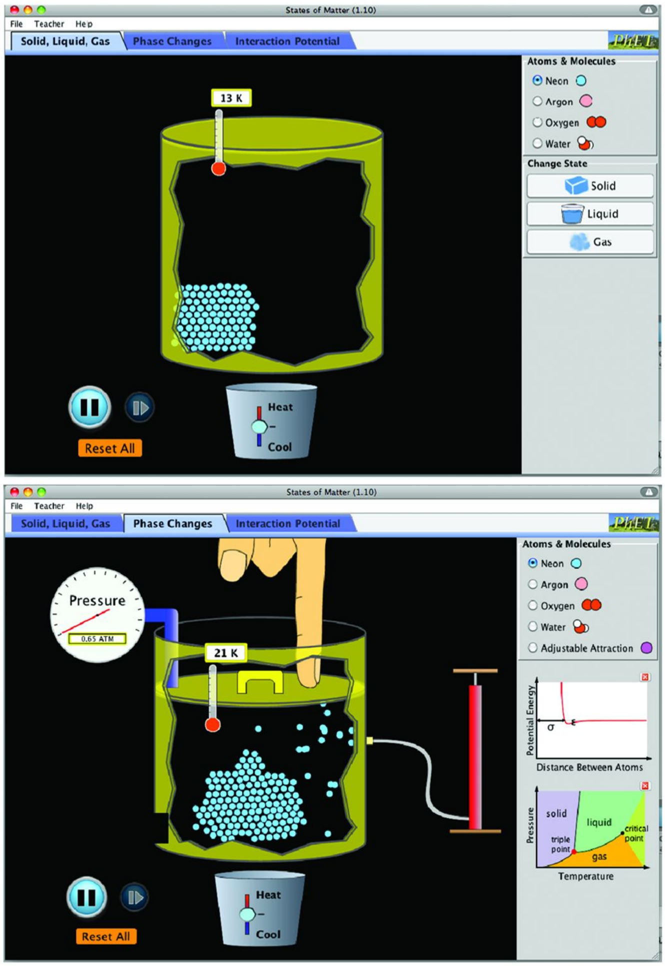

Figure 3. Snapshots of the States of Matter sim, including the "Solid, Liquid, Gas" tab (upper) and the "Phase Changes" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

Interactive

The sims are designed to be highly interactive, allowing users to take actions that directly affect key parameters (e.g. adding or removing heat to change temperature), to use tools to make measurements and observations about the system (e.g. using pressure gauges), and to navigate and modify the environment (e.g. opening the phase diagram, switching tabs, or changing substances).

Dynamic Feedback

In response to each interaction, the sim provides immediate visual feedback of the resulting changes (e.g., readouts increase or decrease in value, molecules slow down or speed up). Feedback is critical to testing ideas and developing a conceptual understanding (*34*). In the "Solid, Liquid, Gas" tab of the *States of Matter* sim, using the 'Solid', 'Liquid', and 'Gas' buttons provides immediate change in the animated, visual representation of the particles in the container, and adding or removing heat results in changes in molecular motions and transitions between phases.

Multiple Representations

The sims provide users with multiple representations – representations that experts use to aid in their understanding. Sims go beyond what is possible in the lab, allowing users to see the invisible (e.g. atoms, photons, electrons). The designs often include multiple representations of a core idea, helping users coordinate across the representations (e.g., graphs, numeric readouts, symbols). This coordination creates a more robust understanding of the concept (*13*).

In the *States of Matter* sim, users see the motion, spacing, and arrangement of atoms or molecules in a substance. The core concept of phase is represented through this dynamic animation, the label on the 'Solid', 'Liquid', and 'Gas' buttons, and the position on the coordinated phase diagram.

Allow Actions

Sim designs allow actions that are difficult or impossible in the real world, but are pedagogically powerful for student learning (e.g. slowing down time, directly manipulating individual atoms or subatomic particles, shooting individual photons). In the "Phase Changes" tab of *States of Matter*, students can directly manipulate atom interaction strength. This feature allows students to explore how interaction strength affects the state of matter through direct observation of the resulting behavior of the atoms.

Intuitive Interface

Our sim designs create an intuitive user interface – one that is useable without instruction. We have assembled a collection of design approaches that students find intuitive to use, drawing from work in education technology (*32*, *37*) and our observations of students using sims (*35*, *36*). We use common controls (e.g. radio buttons, check boxes, sliders, buttons), and often leverage intuitions students bring from real-life experiences to cue the availability of click-and-drag action – using, for instance, handles to signify grab-able objects and buckets to hold drag-able objects. We also leverage intuitions from other common computer programs

– e.g. using the ideas of "minimize", "expand", and "close". PhET sims use minimal words, and these words are carefully chosen. The words are generally not directions, but labels for the various controls – chosen to have clear meaning for the student or as a technical term for which we want the student to develop an operational definition through exploration. In the "Phase Changes" tab of the *States of Matter* sim, students easily spot the cues for click-and-drag action, using the bicycle pump to add more molecules and the handle to change the size of the container.

Implicitly Scaffold

As described above, implicit scaffolding is central to our sim design. In the *States of Matter* sim, examples of perceived affordances include adding or removing heat, changing container size, or adding molecules. In the "Solid, Liquid, Gas" tab, the three button controls are labeled 'Solid', 'Liquid', and 'Gas', cuing students that these terms are important and enabling them to easily jump to each state and correlate the vocabulary with visual representations of particulate-level behavior. These buttons immediately focus student attention on the most important aspects of the chemistry concepts presented in the sim.

Real World Connections

Where possible, sim designs connect to students' everyday life experiences. We adopt this approach with several goals in mind: 1) to reduce cognitive load and cue intuitive interaction (*25*, *33*), 2) to build connections to students' prior knowledge and understanding (*26–29*), and 3) to increase motivation by making the context more relevant to students' experiences and cuing their natural curiosity. In the "Phase Changes" tab of the *States of Matter* sim, students use a bicycle pump to add more particles to the container. The pump cues the desired interaction and helps students interpret what is happening in the sim with less cognitive effort by transferring what they know about bicycle pumps. Inclusion of water in *States of Matter* provides a familiar substance for students and a connection to student's everyday life experiences with ice, liquid water, and water vapor.

Game-like

Learning requires students to do significant amounts of work. Through our sim designs, we aim to create a fun, engaging environment, which triggers curiosity and a sense of challenge and motivates students to interact and explore substantially. Sims motivate student engagement in two ways. 1) Students readily perceive that they have a great deal of control and flexibility over the learning process. This degree of control, or choice, is one of the "game-like" aspects of sims that motivates exploration and productive play (*38*). 2) Use of implicit or explicit challenges, goals, or games draws students into a mode of "figuring things out", which leads to exploring, explaining, and seeing their own understanding improve as they make use of the feedback from the sim. Even when sims lack an explicit challenge or game, students will sometimes create one for themselves. For example, in the "Phase Changes" tab of the *States of Matter* sim, students create games around blowing the lid off of the container, which is productive for exploring the conditions that increase pressure in the system.

Design Process

The PhET sim design process is grounded in education research. The learning goals and initial designs are guided by research on how people learn, research on student conceptual understanding, and research on educational technology. Student interviews inform the sim designs and contribute to the research base. The steps in our design process are highly iterative: for instance, we interview students on early versions of sims to resolve open design questions and issues, resulting in multiple redesigns. In this section, we describe each step of our sim design process.

Learning Goals

The design process begins with the selection of the topic. We prioritize topics for which sims have the potential for large impact in science education. Our selection criteria include: Evidence of student difficulty; alignment with the affordances of sims; connection to real-world contexts; and potential for widespread use. Each sim is guided by content-specific learning goals as well as our general design goals. The content goals are further informed by relevant findings from science education research. Many of the chemistry sims, for example, are designed to address learning goals related to the particulate nature of matter (*39*).

Initial Design

A team – consisting of content experts, education researchers, teachers, interface experts, and software developers – designs each sim. The team creates a storyboard for the sim based on the learning goals. The storyboard provides the look and feel of each sim tab, includes the underlying model, and describes user scenarios – what should happen when the student interacts with the sim. Once the team resolves any design issues, the software developer begins to program the sim. The process of development often generates unforeseen issues to consider. The initial design and development process typically takes 2-6 months to complete.

Student Interviews

Student interviews are the next step in the sim design process. Each interview informs the design of the sim and contributes to the research base. We use a think-aloud format in which students are asked to express their thoughts as they explore the sim. The interviewer only speaks to remind the student to talk (e.g., "What are you thinking now?") or to ask for clarification (e.g., "What did you just say?"). Through these interviews, we seek to answer a number of design questions: Does the sim engage students in exploration? Is the interface intuitive? Do students use the controls in productive ways? Do students correctly interpret the representations and feedback provided by the sim? Are students able to achieve the learning goals of the sim? After multiple rounds of interviews – from 2-6 interviews each round – the design team examines the interview findings and makes design adjustments.

Our interviews have shown that expectation can influence how students explore the sims. Students who do not feel they understand the topic in the sim are more likely to engage in exploration and try to *learn* from the sim. Students who feel they already understand or have already covered the topic are more likely to try to recall the concepts and use the sim to demonstrate or confirm what they already know (*35*, *36*). Consequently, we interview students who have had little to no formal instruction on the sim topic and who are or will soon be the target audience for that sim – for example, we recruit students in the first semester of General Chemistry to test a sim on a second semester topic.

Redesign

The interviews can uncover student interpretations of representations in the sims that differ from those intended. Our redesign of the *Molecules and Light* sim (Figure 4) provides an example of how interviews inform our design process. This sim was designed to allow students to explore how light interacts with molecules in the atmosphere. Our initial design included a spectrum key to illustrate the energy range of each type of light. In an interview on this sim, the student began by using the radio buttons in the control panel to change the molecule. After selecting different molecules, he said that he was confused about the lack of change in the spectrum as he changed the molecule. He was using his prior experience to interpret the spectrum key as emission spectra. The student also did not immediately notice the slider that turns on the light source. To address these issues, we removed the spectrum key and added a "Show Light Spectrum" button that opens a window with the light spectrum. We also increased the size and changed the shape of the slider handle, and removed the "Lower" and "Higher" buttons to focus student attention on the most productive actions within the sim. Further interviews showed that these changes were successful; students effectively used and made sense of the spectrum key and readily found the light source slider.

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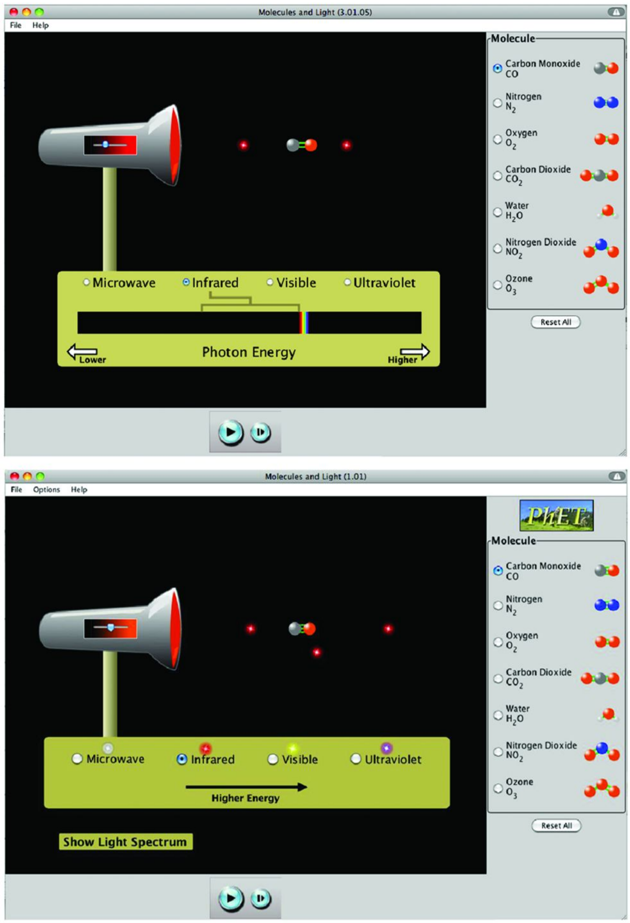

Figure 4. Snapshots of an early design of the Molecules and Light sim (upper) and the redesigned version (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

Final Design

Once our redesign process results in a highly effective sim – that is, students are able to readily achieve the learning goals in interviews without intervention – we reach the final step of the design process, where the final redesign is published to the PhET website. But no sim design is ever completely final. As millions of people around the world use the sims, we receive feedback and suggestions for new features via phethelp@colorado.edu. We collect this user feedback, addressing any bugs immediately and redesigning and republishing sims as funding, resources, and priorities allow. We also revisit the designs of older PhET sims as our design principles evolve.

Part 2: Design Challenges

The PhET Interactive Simulations project began as the "physics education technology" project. While our design principles are largely derived from work on physics sims, we find that the same goals and principles can apply to sims for other science disciplines. Yet we also encounter design challenges specific to each discipline. The process of investigating design solutions to these challenges has served to expand our toolbox of design approaches and to advance our understanding of effective sim design.

A primary goal of chemistry education is for students to develop a new, particulate view of the world. For instance, we want students to be able to visualize the motion of H_2O molecules in a glass of water. But, without the ability to directly observe the particulate nature of matter, students must take the concept of molecules on faith. In contrast, many concepts in introductory physics are more tangible; PhET physics sims often use familiar situations, such as people on a seesaw, to build on the prior experience of students. Many of the challenges we encounter while designing chemistry sims are traceable to the nature of the concepts in chemistry – e.g., the necessity of a symbolic language to coordinate across macro and micro scales, or the emphasis on microscale properties to explain macroscale observations (*39*, *40*).

In this section, we describe some of the challenges of designing interactive chemistry sims, and solutions we have utilized. Throughout, we include results and excerpts from previously published (*35*, *36*, *42*) and unpublished student interviews to illustrate how interview results inform PhET design choices. Each student interview consisted of a think-aloud segment, where students were asked to interact – "play" – with the sim, while audibly verbalizing their thoughts. During this segment, students were not told *how* to interact with the sim – no specific tasks or goals were told to the student. The interviewer did not answer any student content or sim-related questions, and only spoke to ask for clarification of a student comment if it was unclear, to prompt a quiet student to continue speaking or to give a neutral indication that a student's comment was heard. Following the think-aloud segment, interviews typically included a post-question segment – where the interviewer asked the student verbal questions about concepts and particular attributes of the sim design, to which students responded verbally. Interview results described here are based on our observations of the think-aloud segment only, unless otherwise noted. All interviews were video and audio recorded.

Animated and Interactive

Chemical processes are dynamic in nature. Animations have proved useful for helping students visualize the dynamics of chemical processes (*5*, *10*). With a goal of engaging students in inquiry, the challenge becomes designing chemistry sims that are animated *and* interactive. We have found that starting a sim with an animated feature can discourage student exploration (*35*). Here, we compare two

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PhET chemistry sims to illustrate how the learning goals influence the emphasis on animation or interactivity within a design.

The *Reactants, Products and Leftovers* sim (Figure 5) was designed to help students develop a conceptual understanding of limiting reactants. In the "Sandwich Shop" and "Real Reaction" tabs, students can change the amounts of reactants and immediately see the effect on the amounts of products and leftovers. The sim gives a before and after snapshot of the reaction to enable students to directly compare cause and effect. This sim is interactive, but it does not show the dynamics of the reaction – doing so would interfere with the immediate feedback of changing the reactant amounts.

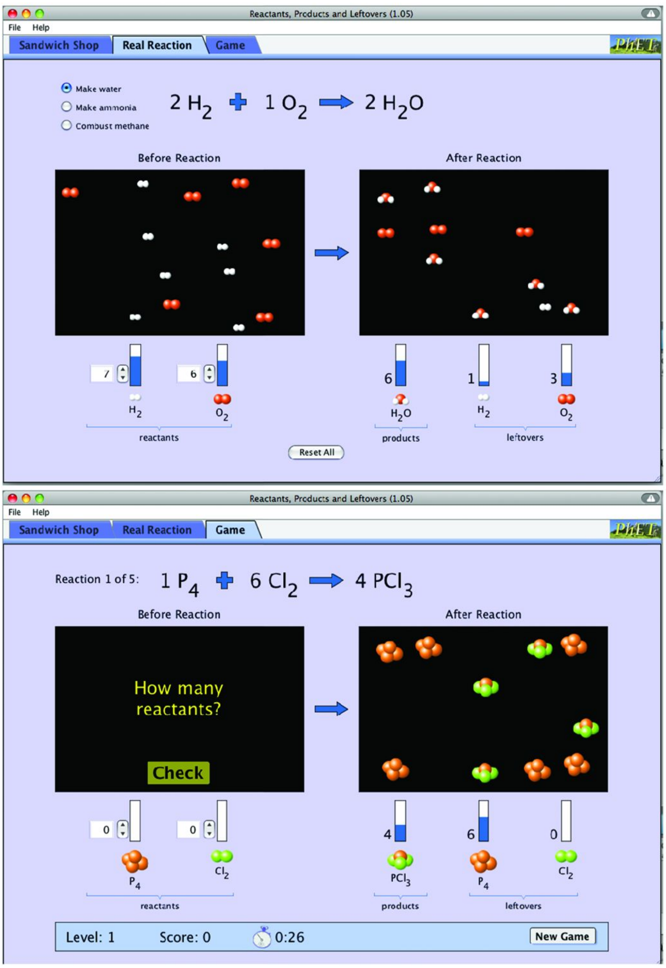

Figure 5. Snapshots of the Reactants, Products and Leftovers sim, including the "Real Reaction" tab (upper) and the "Game" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

In the *Salts and Solubility* sim (Figure 6), the main learning goal is for students to recognize the dynamic nature of solubility equilibria. Students can add different salts to water and observe how the salts dissolve or precipitate. Again, the design choices were driven by the learning goals. The "Table Salt" and "Slightly Soluble Salts" tabs emphasize the visualization of the equilibrium process and limit the interactivity to adding salt and adjusting water levels. The "Design a Salt" tab allows students to design their own salts. This sim was used in a study by Jones et al. (*41*) to investigate the effect of interactivity on student learning. One group of General Chemistry students used the sim as designed, while another group used a screen-captured animation of the sim. We suspect that the animated focus of the *Salts and Solubility* sim is one possible explanation for the lack of significant difference in learning gains between the groups.

Many of the PhET chemistry sims include interactivity with animated features. In the *States of Matter* sim, for example, students can control the amount of heat *and* observe the how the particles behave in response. Part of the design process for each chemistry sim is deciding whether to emphasize the process or the outcome, and then deciding how to use animation and interactivity to address the learning goals.

Continuous and Discrete

Central to the design of PhET sims is the ability for students to easily change a relevant parameter and immediately observe effects. Sliders can be particularly effective tools for allowing this type of interaction. Their usefulness extends to chemistry sims, with some additional considerations.

A possible concern with sliders in chemistry sims is that students are allowed to continuously vary properties that are discrete in the real world. In response to this concern, we often divide the chemistry sims into two sections: specific and general. The specific section allows students to compare and contrast real atoms, while the general section allows students to customize the properties of atoms. In the *Atomic Interactions* sim (Figure 7), students can compare the potential energy diagrams of specific diatomics and then adjust the attraction between generic atoms. The order is reversed in the *Molecule Polarity* sim (Figure 8), students can change the electronegativity of generic atoms and then investigate the polarity of real molecules.

We interviewed five students in General Chemistry I on the *Molecule Polarity* sim. During interviews, students used the sliders in the "Two Atoms" and "Three Atoms" tabs to explore the effect of electronegativity on the magnitude and direction of the molecular dipole. After comparing real molecules in the "Real Molecules" tab, students returned to previous tabs to recreate the cases from the "Real Molecules" tab (e.g., creating a water-like molecule), found molecules that do not follow common trends (e.g., ozone), and predicted the direction of the molecular dipole before checking with the sim. During the post-question segment of these interviews, we investigated how students interpreted the continuous

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slider by asking students if it was possible to change the electronegativity of an atom. Students responded with comments including: "*I assume that each, um, each element has its own electronegativity…I assume when you're sliding this* [electronegativity slider] *it's just changing the identity of the atom*" and "*I don't think in real life you can do it* [change the electronegativity of an atom]."

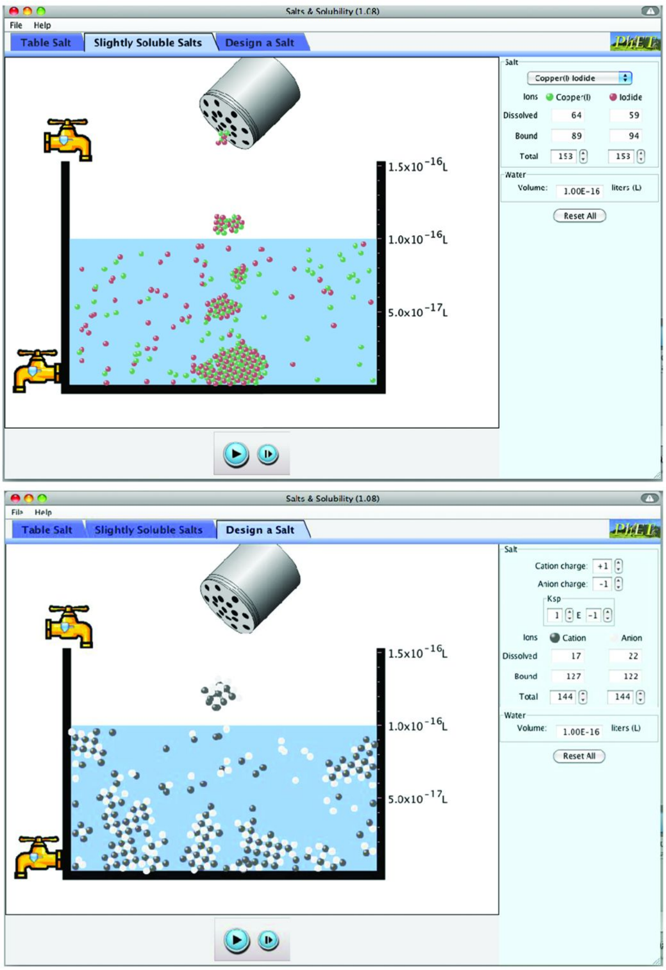

Figure 6. Snapshots of the Sugar and Salt Solutions sim, including the "Slightly Soluble Salts" tab (upper) and the "Design a Salt" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

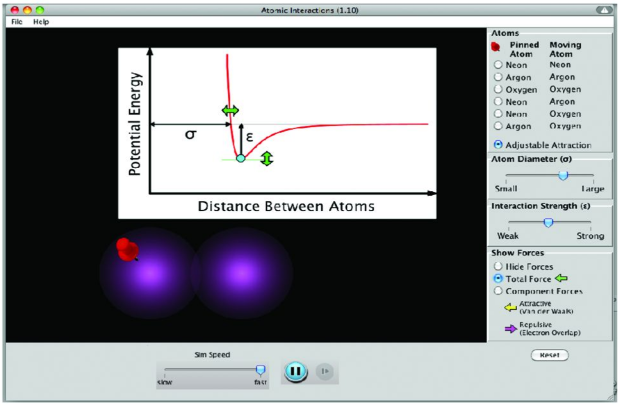

Figure 7. Snapshot of the Atomic Interactions sim. Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

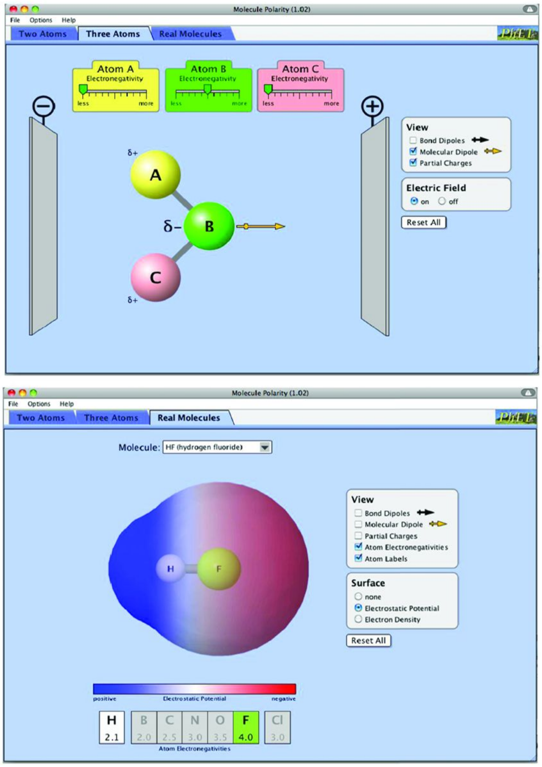

Figure 8. Snapshots of the Molecule Polarity sim, including the "Three Atoms" tab (upper) and the "Real Molecules" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

Another challenge arises with the use of chemistry equations, which tend to *summarize* the process (e.g., A → B) rather than *describe* the process. In the *Acid and Base Solutions* sim (Figure 9), students can vary the strength of a generic acid (HA) and observe the effect on the particles in solution. A primary learning goal for this sim is understanding the effect of strength; thus, in the sim design we chose not to show the equilibrium process in favor of immediate feedback on the effect of strength. During 11 interviews with General Chemistry I students we found that the students tried to reconcile their observation that increasing acid strength resulted in less acid (i.e., HA) in solution. While this was a useful question for students to explore, we observed that the design choice to show only the equilibrium condition – and not the dynamic process to get to equilibrium – did limit students' ability to fully explore and make sense of these observations. A future redesigned version of the sim may include a 'reaction progress slider' to enable increased exploration.

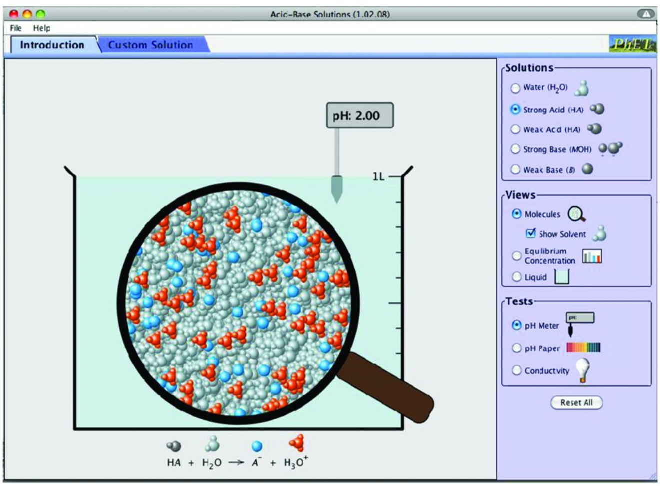

Figure 9. Snapshot of the Acid and Base Solutions sim "Introduction" tab. Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

These observations suggest that using sliders in chemistry sims is productive for engaging students in exploration and sense making. Our approach of providing students with general, customizable systems together with discrete, real-world examples supports both comparing distinct cases and discovering trends, as well as directly interacting with a parameter to determine its effect. The challenge is to integrate this design tool in ways that aid student understanding and avoid misinterpretation.

Macro and Micro Scales

Another challenge for chemistry sim design is how to indicate scale in a way that enables students to effectively link the macro and micro levels of chemistry. Here, we describe some of the approaches we have used to address scale.

The *Salts and Solubility* sim (Figure 6) uses a mixture of scales to connect the tangible act of shaking salt into water with the particulate visualization of salt dissolving in water. It also uses an image of a faucet to indicate that water can be added to the beaker. Water is shown as continuous to draw on student experience and to focus student attention on the behavior of the ions. The small volume of the container is indicated by the tick marks along the side of the beaker. While some animation developers caution against mixing macro and micro images (*2*), previous analysis of interviews with PhET sims has shown that students recognize when a difference in scale is unrealistic (*36*). Though we have found no indication of confusion regarding scale differences during interviews, it is possible that there are contexts in which this issue will arise in the future. As we design new chemistry sims, we will continue to be attentitive to student comments regarding scale.

A related challenge is how to represent the large number of particles that are responsible for observable macroscopic behavior. An early version of the *Acid and Base Solutions* sim (Figure 10) provides an example of how students respond to different representations. In this early sim version, the particles in solution were shown quantitatively by bar graphs and qualitatively by dots in the beaker. We interviewed eight students in General Chemistry I to determine the effect of each representation (*42*). Half began the interview with the bar chart showing, and half began with the particles in the beaker showing. The initial reactions of both groups were quite different. Students in the ‘bar chart’ group were noticeably overwhelmed upon first seeing the sim. One student put both hands in the air and said “Lot of things at once!” upon first seeing the sim. Students from the ‘particles in beaker’ group had no negative responses upon seeing the sim. We interpreted these interviews as indicating that students could benefit from better implicit scaffolding in the sim, to encourage engagement at the start and support coordination of the graphical and pictorial representations.

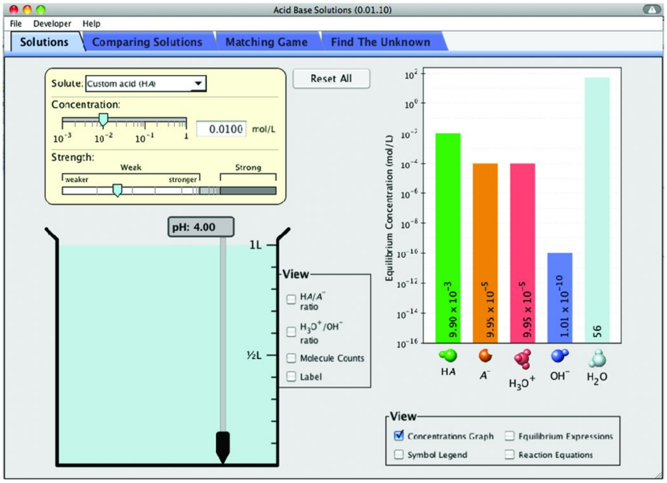

Figure 10. Snapshot of an early design of the Acid and Base Solutions sim. Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

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We used the results from interviews on the early *Acid and Base Solutions* version to inform a redesigned version of the sim (Figure 9). In the redesigned sim, the start-up screen focuses student attention on the concrete representation of the beaker. As opposed to mixing scales, this sim includes tools that allow students to explicitly move across scales within a single tab. Students can use lab tools to measure properties of the macroscopic solution (pH meter, pH paper, conductivity meter) and they can use a magnifying glass to view the particles in solution. The redesigned *Acid and Base Solutions* sim also shows a model of the actual particles – where each particle image represents a concentration value for that particle – allowing students to connect the visualization to the chemical reaction. The design choice of using particle images to represent a concentration value results in a more conceptual view, rather than an exact count of the particles. For other topics we take a different approach, for example, in the *Salts and Solubility* sim each image represents one particle.

Another approach is to describe a single chemical process on multiple scales. In the *Sugar and Salt Solutions* sim (Figure 11) we use tabs to explicitly identify the scale. This sim was designed to help students visualize what happens when sugar and salt are added to water. In the "Macro" tab, students can only do what is possible in a real laboratory: for example, they can add salt to water and measure the conductivity of the solution. In the "Micro" tab, students can compare how salt and sugar dissolve in water. Again, we elected to show water as continuous in this tab to focus student attention on the behavior of the solute particles. In the "Water" tab, students can explore the role of water in the dissolution process: for example, they can drag in a crystal of salt and observe how the polar water molecules reorient around the ions. Each tab provides a different view of the dissolution process.

We interviewed 12 General Chemistry I students with the *Sugar and Salt Solutions* sim. One student commented on the progression of tabs at the end of the interview: "*I guess that's how in my mind it progressed, you know, what happens, why does it happen and how…And I guess the what is the macro* [tab], *the why would be the micro* [tab] *and how would be how water molecules break them* [salt and sugar] *apart* [in the "Water" tab]." This student had determined that the purpose of the tabs was to provide three different viewpoints for understanding the process of dissolution.

These examples illustrate a range of techniques used to represent scale in PhET chemistry sims, based on the context and student interpretations. We use numbers or objects to cue scale. We use tools, such as the magnifying glass, to allow students to move among scales within a single tab. We use tabs to explicitly identify and allow a shift from one scale to another. We expect that our design toolbox will continue to expand as we address new chemistry topics.

Two- and Three-Dimensional Representations

While many chemistry learning goals can be achieved with two-dimensional representations, some learning goals are best addressed using three-dimensional

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representations. We have used two different approaches to address the challenge of designing sims with three-dimensional representations. One approach involves embedding *Jmol* – an open-source three-dimensional molecule viewer (*43*) – into an otherwise two-dimensional sim. The second approach is to design the entire sim with three-dimensional representations. The approach utilized depends on the learning goals of the particular sim.

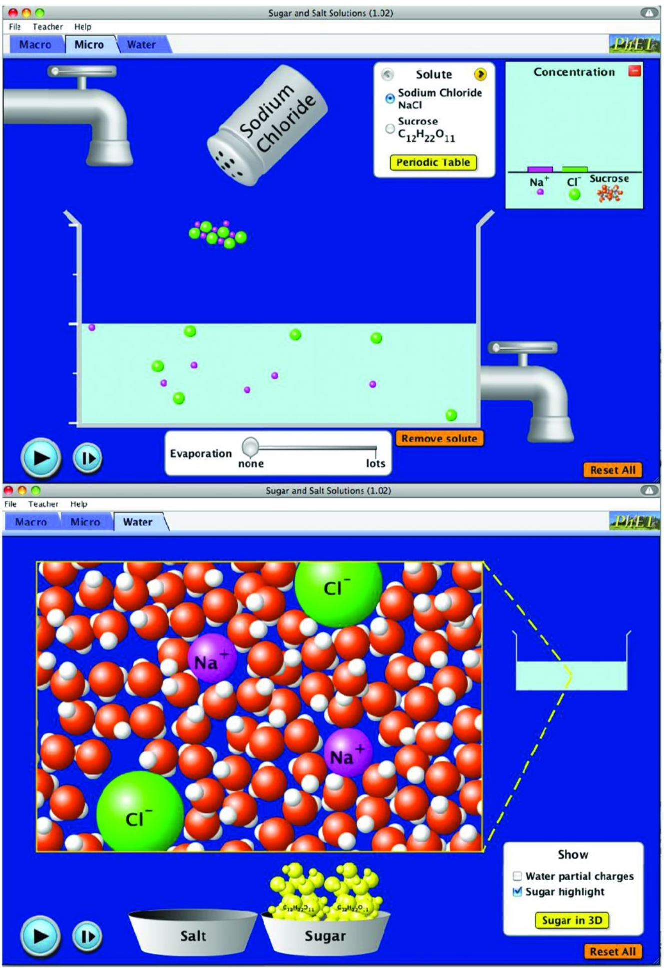

Figure 11. Snapshots of the Sugar and Salt Solutions sim, including the "Micro" tab (upper) and the "Water" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

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The learning goals of the *Build a Molecule* sim (Figure 12), for example, center on understanding chemical formulas and relating multiple representations of molecules. After students make a two-dimensional molecule in the sim, they have the option to open a *Jmol* window and to compare two-dimensional and three-dimensional representations. In the *Molecule Polarity* sim (Figure 8), one of the goals is for students to predict the polarity of molecules using bond polarity and molecular shape. The "Real Molecules" tab uses the capability of *Jmol* to show the bond and molecular dipoles of three-dimensional molecules along with the electrostatic potential surface – after students have explored two-dimensional representations of these concepts.

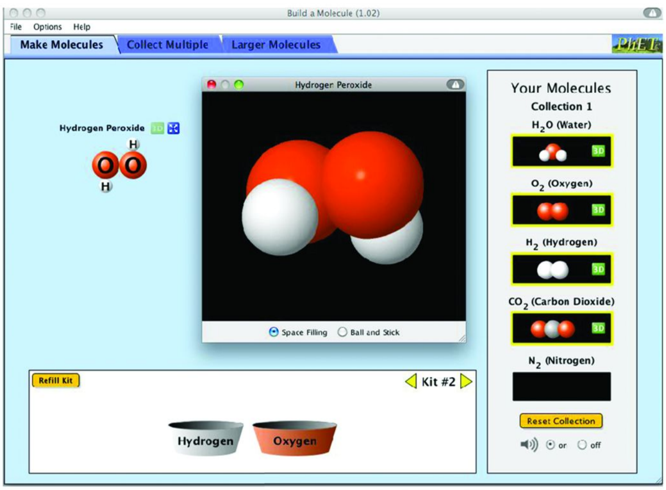

Figure 12. Snapshot of the Build a Molecule sim Make Molecules tab. Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

The *Molecule Shapes* sim (Figure 13) is designed entirely with three-dimensional representations. In the "Model" tab of *Molecule Shapes*, students can interact with a model molecule that changes geometry based on the addition and removal of terminal atoms and lone pairs. By designing the sim using three-dimensional representations, students are able to see and interact with the molecule's change of geometry in direct response to the distance between atoms and lone pairs. In the "Real Molecules" tab, students can compare geometries between real molecules and the model molecules. This feature allows students to determine the effect of lone pairs on geometry and compare geometries across real molecules.

These sim examples demonstrate our selective use of three-dimensional representations. This selective use of three-dimensions is influenced by research on multimedia design showing that visual complexity can interfere with student learning (*32*). For example, our use of three-dimensional representations has largely been focused on single molecules where complexity of the three-dimensional representation is limited.

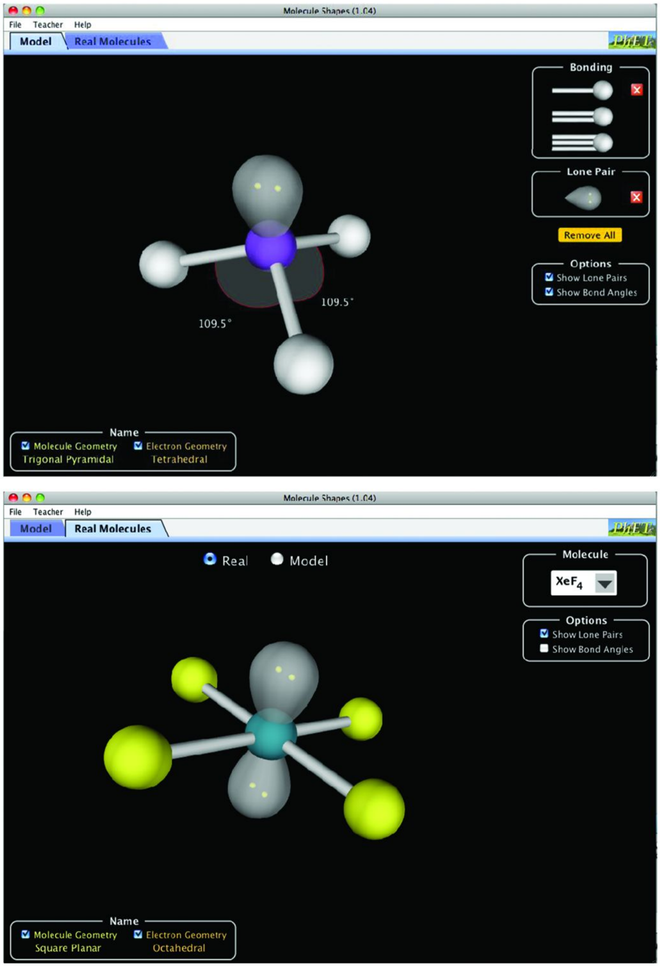

Figure 13. Snapshots of the Molecule Shapes sim, including the "Model" tab (upper) and the "Real Molecules" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

Implicit Challenges and Explicit Games

Understanding chemistry requires being able to manipulate abstract symbols, such as chemical formulas and equations, which represent phenomena across multiple scales (*39*, *40*, *44*). A balanced chemical equation, for example, represents both the conservation of mole ratios between reactants and products and the conservation of atoms as reactant molecules reorganize into product molecules. Mastering symbolic representations more closely resembles learning a language than learning a scientific concept (*45*). PhET sim designs generally utilize *implicit* challenges (with optional goals but no score) or *explicit* games (with correct answers and scores), or both. We have found that designing with emphasis

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on implicit challenges and explicit games can increase student engagement, particularly with sims that rely heavily upon symbolic representations.

The *Balancing Chemical Equations* sim (Figure 14) provides a typical example of an explicit game in a PhET sim. The “Introduction” tab allows students to explore the concept, while the “Balancing Game” tab allows students to apply the concept and test their understanding. Learning with the game is further scaffolded by the inclusion of levels of increasing difficulty. After students enter an answer, the game provides feedback and allows students to try again if needed. After a second incorrect attempt, students are shown the correct answer.

In interviews with the *Reactants, Products and Leftovers* sim (Figure 5), we observed increased engagement from use of the explicit game. In the “Sandwich Shop” and “Real Reaction” tabs of the sim, students can change the amounts of reactants and observe the effect on the amounts of products and leftovers. In the “Game” tab, students are given the reactant amounts and must predict the amounts of products and leftovers. We asked 15 introductory chemistry students to use this sim and found that most students spent a few minutes exploring the “Sandwich Shop” and “Real Reaction” tabs. The “Game” tab, however, proved to be highly engaging – students spent an average of 40 minutes, unprompted, playing the game.

In seven interviews with middle school students using the *Build an Atom* sim (Figure 15), we observed the explicit game providing motivation for students to succeed in understanding the sim content. In the “Build Atom” tab, students can build atoms with protons, neutrons and electrons, and view readouts of the symbol, mass and charge. Students can later test their understanding in the “Game” tab; in the first level, for instance, students are given the number of protons, neutrons and electrons, and must find the element in the periodic table. In general, the students used the “Build Atom” tab to explore the structure of atoms but did not focus on the readouts. When playing with the “Game” tab, students returned to the “Build Atom” tab to build the atoms. When motivated by getting the correct answer in the game, these students used the readouts to develop rules for element, mass, and charge, and their locations in the element symbol.

Another strategy is to encourage students to attend to specific challenges in the sim. In this implicit challenge design, students can choose to work toward these goals or create their own goals. This strategy is used in the *Build a Molecule* sim (Figure 12), where the goal in the “Make Molecules” tab is to build each of the molecules listed in the collection area. Students can also build other molecules, but the included goal provides a direction for their play and focuses attention on interpreting the chemical formulas. The challenge in the “Collect Multiple” tab is to collect multiples of the molecules, focusing student attention on interpreting coefficients. We interviewed 14 middle school students and found the instant feedback provided by the sim helped refine their understanding of chemical formulas. In this example, an 8th grade student used feedback provided by the sim – in the form of the appearance and lack of appearance of a molecule name – to help her build CO_2, a goal molecule.

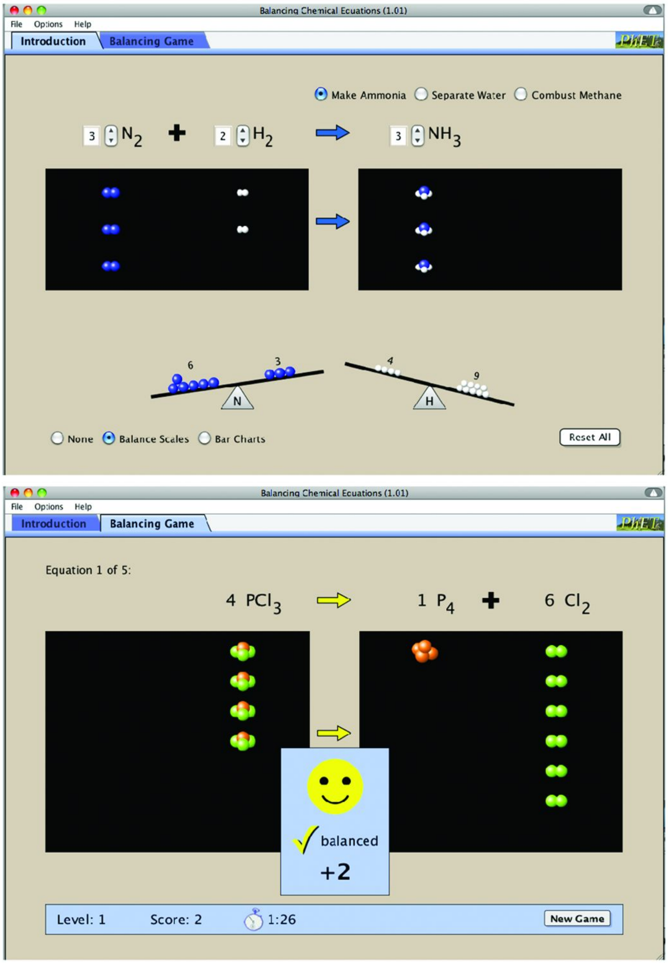

Figure 14. Snapshots of the Balancing Chemical Equations sim, including the "Introduction" tab (upper) and the "Balancing Game" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

[Student puts together C-O.]

Student: *Carbon monoxide, ooh.* [Adds a second O to the O in CO, making COO. No molecule name appears.]

Student: *I put that on wrong.* [Breaks apart atoms.]

Student: *See they* [atoms in the molecule] *have to be a certain way.* [Adds O's to the C. 'Carbon Dioxide' appears above molecule.]

Student: *There, that's better.*

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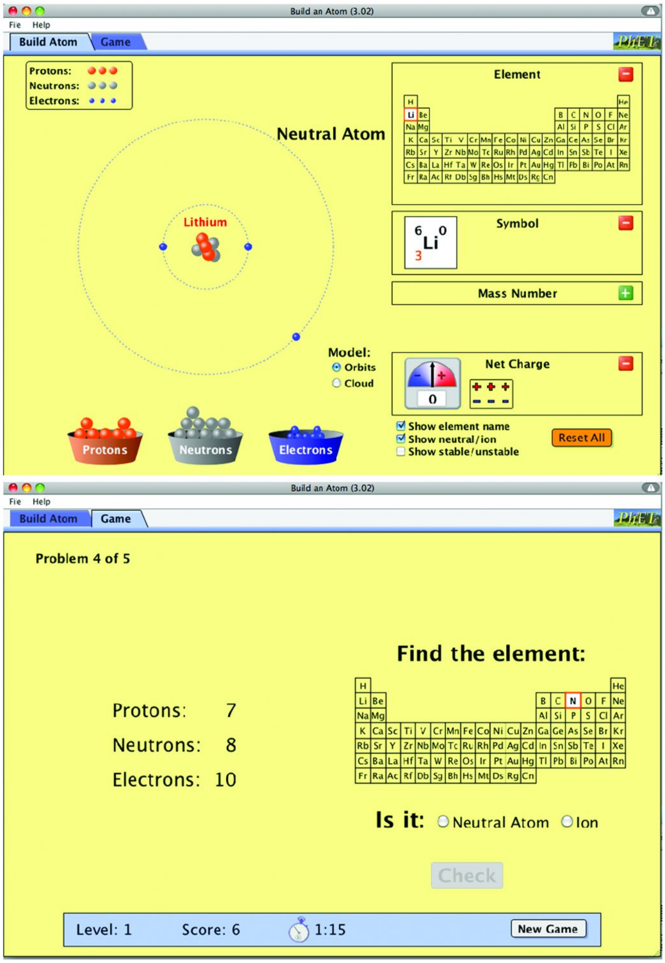

Figure 15. Snapshots of the Build an Atom sim, including the "Build Atom" tab (upper) and the "Game" tab (lower). Courtesy of PhET Interactive Simulations, University of Colorado Boulder.

Student engagement, enjoyment, and motivation are among the overarching goals for our sims. Among other reasons, these factors increase the likelihood that students will devote the time and effort to making sense of the science ideas. Historically, many of our physics sims provided natural built-in challenges and puzzles that sparked curiosity and provided motivation to explore (*30*, *35*, *46*). Some science topics and concepts are, however, less naturally engaging. The examples above demonstrate that building in explicit games and implicit challenges can be highly motivating for students and can drive additional sense making of concepts, such as helping students interpret symbolic representations in chemistry.

Qualitative and Mathematical Models

Chemistry concepts are nuanced, with overarching trends and interesting exceptions. The absence of a mathematical model poses a challenge in developing some chemistry sims. For example, during development of the *Build a Molecule* sim (Figure 12), with which students can make molecules from atoms, we searched for quantitative ways to model chemical bonding. One option was to use rules (e.g., carbon can make four bonds), but the exceptions (e.g., CO) outnumber the rules. Our solution was to productively constrain the atoms available through the use of kits and to include a database of over 9000 molecules for all possible combinations of the available atoms. Each time a student drags one atom near another in the play area, the sim searches the database to instantly determine if the result is a real molecule or is part of a real molecule. As the PhET project has moved into biology and geosciences, we have encountered similar challenges with topics – such as plate tectonics or protein synthesis – which lack straightforward mathematical models, but have overall qualitative behaviors that represent key conceptual ideas within these disciplines.

Discussion and Conclusion

In this chapter, we presented an overview of our philosophy and approach to chemistry sim design, highlighting the chemistry-specific challenges that emerged over the course of this work. Through sim design, we seek to not only support student content learning, but to simultaneously address scientific process knowledge and skills, and to support affective goals. We also seek to support easy integration with a variety of teaching approaches, including student-centered pedagogy. Developing sim designs that satisfy this combination of goals has proven to be achievable, through creative solutions to design challenges.

The interactivity and dynamic feedback features of sims have been particularly challenging to design, but are critically important to achieving these goals. These features support student content learning, and are essential to addressing scientific process goals. When successful, we observe the richness of the interaction-feedback cycle, providing students with the context and ability to explore and make sense of complex chemistry topics. Often, these features give students control over tangible physical changes – developing their ideas about what and how to investigate in real life – while providing tools or visualizations only available in virtual environments. Through these interaction opportunities, students are participating both in the process of creating and controlling these virtual systems and in the process of discovering knowledge and creating their own understanding.

We find that the challenges encountered in designing chemistry sims highlight and reflect what makes chemistry interesting and challenging as a science. It is challenging to: Explain macroscopic behavior in terms of submicroscopic interactions; to represent physical processes in terms of symbolic and pictorial representations; and to use contrasting real-world examples to identify trends and develop models, in the face of many exceptions.

Two design processes have been particularly useful in managing these challenges, guiding our development, and deepening our understanding of sim design and use. First, developing learning goals for each sim – both the overarching goals described above and the sim-specific content learning goals – clarifies what is needed from each sim. We consistently find it useful to use these learning goals to drive the initial sim design and to refer back to them when faced with design choices or challenges. In addition, student interviews have been an invaluable resource for evaluating design elements for ease-of-use, accurate and consistent interpretation by students, and engagement – all of which are necessary to reach the design goals. With the results of each interview feeding back into the sim design and our design research base, these interviews have significantly advanced our understanding of effective sim design as well as our understanding of how students engage with and learn from sims.

Extending and adapting our design philosophy and approach to create interactive chemistry sims has been and continues to be challenging. These challenges – for the PhET team and for the community of simulation researchers – drive creativity, and provide new insights into simulation design and student learning. The result is an expanding toolbox of design approaches and a deepening understanding of simulation design and the teaching and learning of chemistry.

Acknowledgments

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Chapter 6

Animation or Simulation: Investigating the Importance of Interactivity for Learning Solubility Equilibria

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The aim of this mixed-methods study was to investigate the effect of interactivity when learning from a computer visualization of the dynamic nature of solubility equilibria. Forty-two general-chemistry and high-school students completed a computer lesson on solubility equilibria. Half the students were randomly assigned to complete an interactive solubility equilibria simulation and the other half were assigned to complete a screen-captured animation of the same simulation. All students completed an open-ended questionnaire on the dynamic nature of equilibrium and a conceptual test on solubility equilibria before and after the implementation, and a cognitive load questionnaire and an attitude questionnaire just after working with the visualization. Only the open-ended questionnaire showed changes in mental models of dynamic solubility equilibria. The analysis showed that the students tended to use molecular features significantly more frequently ($p < 0.05$) in their mental models after completing the computer lesson than before. However, no significant difference ($p = 0.690$) was found between the animation and simulation groups. A negative correlation between perceived cognitive load of the visualization and the conceptual post-test on solubility equilibria was found, but no difference in perceived cognitive load of the simulation and animation was observed. Regardless

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of the type of visualization used, the majority of the students found the visualization helpful. In the qualitative part of the study, students and instructors were interviewed to gather their opinions on the positive and negative aspects of the visualizations.

Background

Animations are widely used to help learners visualize the molecular level (*1–7*). However, animations have intrinsic problems. They can be misleading and too much can happen at one time, so that learners may not know what is important (*8*). The pacing of an animation is fixed and may be too fast or too slow for individuals (*9*). These factors can lead to high cognitive load (*10*).

Oakes and Rengarajan (*11*) defined simulations as interactive models that encourage learners to learn the content by interacting with and exploring the model, whereas animations are multimedia presentations rich in graphics and sound, but almost never interactive. Simulations offer an interactive learning environment, as opposed to the passive learning environment of an animation. For example, the ability to control variables and view the outcomes can help learners identify relationships and thus enhance understanding (*12*). Pacing can be controlled by the learner and the simulation is usually repeated several times, which may enhance learning (*13*, *14*). Interaction that involves direct feedback on learning has been found to be effective. In a study by Avner, Moore, and Smith (*15*) students completed one of two versions of a computer lesson containing simulations of chemistry laboratory activities. In the first version the students had complete control over the pacing and variables. In the second version, the pacing was controlled by the computer and students were allowed to proceed only when they had carried out the procedures correctly. Students using the second version, which allowed less control and no exploration, but was more highly interactive, performed better on the subsequent laboratory assignment. The reason for their improved learning was attributed to the frequent feedback students received on their choices as they proceeded through the lesson.

Simulations have been used in teaching many chemistry concepts, including molecular dynamics (*16*), chemical kinetics (*17*), solubility equilibrium (*18*), chemical reactions (*19*), and chemistry laboratory practice (*20*). Simulations are viewed by some researchers as more powerful learning tools than animations due to the control a learner can exercise over the program (*21*) and the active involvement required (*22*). Mayer and Chandler (*23*) found that students who controlled the pacing of an animation showed no difference in retention over those who had no control over pacing, but they performed better on a transfer activity, suggesting that they may have developed a deeper understanding of the concepts. Active involvement with a simulation may actually present problems. Rodrigues and Gvozdenko (*24*) found that the more interactive a simulation is, the more the student interacts with it, which may reduce the learning efficiency of the lesson. In addition, a meta-analysis of learner control in computer-based instruction found only a small negative effect size, which implies that student control over the variables and pacing of computer lessons, including simulations, may not be necessary or even helpful (*25*). This study was designed to explore the importance of interactivity in learning from a simulation. The type of interaction allowed in this study was control over the pacing and variables, combined with the opportunity to view the consequences of choices. That is, the feedback came only from the logical chemical outcomes of the choices, not from achieving a correct or incorrect answer.

Theory

Constructivism

The theory that guided this work was constructivism. This theory acknowledges that every learner has unique needs and background knowledge on which to build new learning. It assumes that new knowledge is constructed through interacting with the content. (*26*, *27*). The interactive constructivist model provides a way to apply these ideas to active learning environments (*28*). In the interactive constructivist model interpretations of observations are judged against evidence from nature. The learner develops his or her own conceptions, which are then modified by interactions with others.

Simulations can support an interactive constructivist environment when they are developed using scientific principles. In such an environment learners receive feedback on their interpretations of these principles (*29*). It would appear that a simulation would lend itself better to an interactive constructivist learning environment than an animation, but simulations are more difficult and expensive to produce than animations. This study considered whether animations can also be viewed as an interactive constructionist environment.

Mental Models (Representations)

Mental models are our individual constructions of reality. They are derived from perception, imagination or comprehension and often present themselves as visual images or abstractions (*30*). Visualizing molecular structure and dynamics requires construction of a mental model (*31*). Because these models are complex, open-ended research methods are recommended to identify them (*32*). In addition to written explanations the representations that students create can give us useful information about their mental models (*6*, *33–35*). In this study we applied an instrument that we had developed to evaluate mental models of physical equilibrium by analysis of student writings and representations (*36*).

Cognitive Load

Cognitive load has been defined as the amount of mental effort required by working memory while performing a particular task (*10*). Cognitive load theory (CLT) is concerned with the development of instructional strategies for efficient use of cognitive processes for learning (*37*, *38*). Kalyuga, Ayres, Chandler, & Sweller (*39*) suggest that a learner's prior knowledge determines the cognitive load the individual will experience. Cognitive load can be manipulated by instructional design of learning materials (*40*). Van Merriënboer, Kirschner, and Kester (*41*) suggest that when the appropriate scaffolding, which is defined as provision of support and gradually increasing the students' responsibility to enhance learning, is provided to the learners, intrinsic cognitive load will be reduced. On the other hand, Schnotz and Rasch (*42*) found that reducing cognitive load can even reduce learning if so much information is provided that learners adopt passive learning strategies.

In their theory of multimedia learning, Mayer and Moreno (*43*) make three assumptions about how the mind works in multimedia learning. First, humans possess distinct channels for verbal and pictorial representations (the dual channel assumption); secondly, each channel is limited in the amount of information processed at one time (the limited capacity assumption), and finally, meaningful learning occurs when the learners make connections between these representations (the active-processing assumption). In multimedia instruction that includes dynamic representations such as animations and simulations, fast pacing and too much information on the screen at once can create cognitive overload (*43*). In a simulation, a student must make decisions about what are appropriate changes in variables, creating another challenge that might increase cognitive load. A simulation with many variables and decision points could be much more challenging for a learner than an animation in which an expert presents the student with a desirable path through the material. Mayer & Moreno (*43*) suggest dividing complex animations and simulations into segments and providing prior training in the use of the program as means to reduce the cognitive load of the instruction.

In this study worksheets were used to reduce the cognitive load of the lessons by helping students to focus on the lesson goals (*44*). Students were also assigned to work a simulation or an animation to assess whether the additional options available in the simulation were perceived as increasing or decreasing cognitive load. A subjective method was used to measure perceived cognitive load. A questionnaire measuring the dimensions of mental load, effort, and performance (*37*) of the simulation or animation was completed by study participants.

Content Focus: Physical Equilibrium

Physical equilibrium is a fundamental concept of chemistry that is usually taught before chemical equilibrium, as it is thought to be simpler to comprehend. However, it is commonly viewed as one of the most difficult chemical concepts to learn (*45–47*). The dynamic nature of equilibrium at the particulate level is particularly difficult to learn (*48*). Many learners have misconceptions of the dynamic nature of equilibrium (*49*, *50*), but most of the research on learning about equilibrium has focused on the mathematical aspects (*46*, *51–53*). Therefore, physical equilibrium was chosen as the target content area for this study.

Purpose of the Study

As part of a larger study of the role of computer visualizations in learning chemistry (*36*), differences in student learning and attitudes related to completing either a simulation or animation of physical equilibrium were examined. The research questions for the study were:

- How are mental models of molecular processes held by introductory chemistry students affected by viewing related animations or simulations accompanied by worksheets?
- What differences in mental models, attitudes, and perceived cognitive load are observed when students use an animation instead of a simulation?

Method

Participants

The 42 participants in this study included 32 second-semester college-level general chemistry students and 10 high school students enrolled in a second-year chemistry class. Twenty-one (50%) of the students were male. Twenty-nine students (69%) were Caucasian, six Hispanic, five African-American, and one Asian. Following approval by the university's Institutional Review Board, participants were selected by recruiting volunteers in the chemistry classrooms. The participants all signed consent forms and the parents of the high school students also signed parental consent forms. When the college-level and high-school students were compared with respect to their initial mental models of the dynamic nature of equilibrium, no significant difference ($p < 0.05$) between the groups was found; hence all the students were grouped together.

Research Protocol

During the 12th week of the semester, the general chemistry students completed short demographic forms and the pre-test (CSPrT) at the beginning of their lecture class. The pre-test required about 10 minutes. On the same day, participants were then taken individually to an educational research laboratory containing laptop computers on which either a simulation of solubility equilibrium or an animation of that simulation was available. High school students worked in their actual class setting on computers provided by the researchers. Participants were randomly assigned as individuals to complete either the simulation (Simulation group) or the animation (Animation group) while guided by a worksheet. Students were provided at random with a more-guided or a less-guided worksheet. Participants were allowed to work at their own pace; students took about 35-45 minutes to complete the computer lesson. An open-ended pre-test (OCQ) was used to assess mental models of physical equilibrium and the same test

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was administered immediately following the lesson. Thus, a pre-test – treatment – post-test design was used for two different types of tests. After completing the computer lesson, the students completed the 10-minute post-test (CSPoT), a 5-minute cognitive load questionnaire (CLQ), and an attitude survey.

After the implementation of the study, four students were interviewed as they worked through the simulation or animation to develop a deeper understanding of their mental models about the dynamic nature of physical equilibrium and to probe their interactions with the computer animation or simulation. Four experts (two university instructors and two high-school teachers) and four students, one from each of the categories Animation-less guidance, Animation more guidance, Simulation-less guidance, and Simulation-more guidance, were randomly selected to be interviewed. The interviews were conducted in a think-aloud format and students were asked to explain what they thought while they were working with the simulation or animation. The interviews were audio and video-recorded and took about 20-25 minutes.

The Simulation and Animation

The simulation chosen for this study was the "Salts & Solubility" simulation developed by the PhET Interactive Simulations research group at the University of Colorado Boulder (*54*, *55*). It was selected because it addresses both the mathematical and conceptual aspects of solubility equilibrium and allows students to explore diverse aspects of solubility equilibrium by changing variables and viewing the consequences of their choices. The simulation is a Java applet and is available freely online at http://phet.colorado.edu/en/simulation/soluble-salts.

The simulation has three tabs that take the user to three simulations: "Table Salt", "Slightly Soluble Salts" and "Design a Salt". In each tab, users have a virtual shaker from which they can pour salt crystals into a container of water and watch the dissolving of the ions (represented as colored spheres) in water (represented by a blue background). They may also drain some solution and add water to the existing solution. The panel at the right of the screen includes a counter showing the number of dissolved and bound ions, as well as the total number of ions in the solution, to help students visualize the dynamic nature of equilibrium. Users also have the option of viewing the ions in the solution. A screen shot from the simulation is shown in Figure 1.

The animation of the PhET simulation is composed of three animations that take the student through the three sections in the simulation. The "Table Salt", "Slightly Soluble Salts" and "Design a Salt" simulations were recorded by the researcher as if a user were interacting with the simulation. The student views the same outcomes as if he or she had been operating the simulation, but has no control over the variables (Figure 2). The program, Render Soft CamStudio2.0, was used to capture the animation. Students in the Animation Group watched the three different animations separately. They were allowed to view each animation twice, and to stop, pause and replay the animations as they wished to do.

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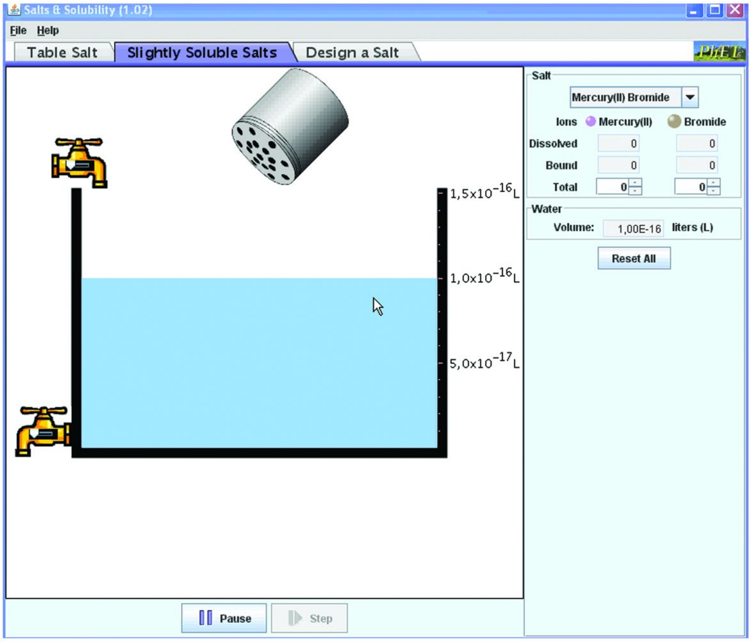

Figure 1. One screen from the "Slightly Soluble Salts" section of the PhET Salts & Solubility simulation. (Courtesy of PhET Interactive Simulations research group at the University of Colorado Boulder.) (see color insert)

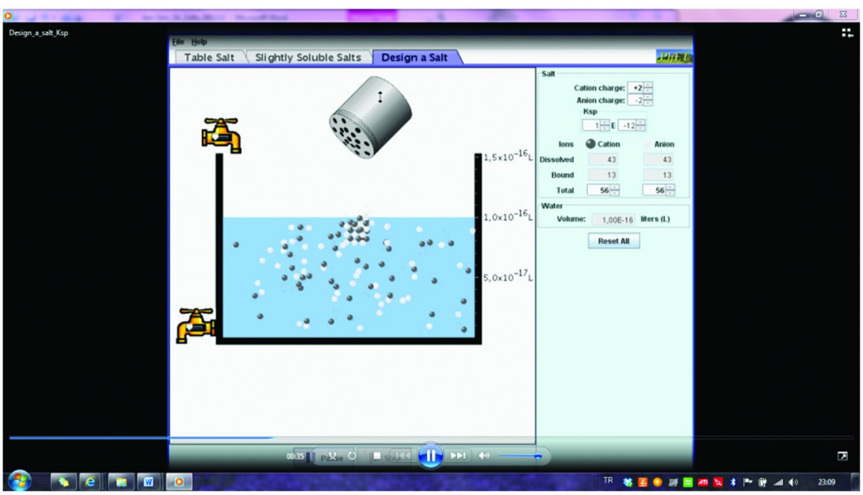

Figure 2. One screen from the "Design a Salt" section of the screen captured animation of the PhET Salts & Solubility simulation. (Original courtesy of PhET Interactive Simulations research group at the University of Colorado Boulder.) (see color insert)

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Tools and Instruments

Open-Ended Conceptual Questionnaire on Solubility Equilibrium

An Open-ended Conceptual Questionnaire (OCQ) was developed to elicit student mental models of the dynamic nature of equilibrium and to assess student ability to transfer their learning to a new system. The questionnaire contains open-ended questions on two topics of physical equilibrium: Liquid-vapor and solubility equilibria. Students were asked to describe the equilibrium conditions both at the macroscopic and particulate levels in either words or drawings. The same OCQ was given before and after the implementation. For solubility equilibrium students were presented with a drawing of a system consisting of molecular iodine being added to water. The liquid-vapor system consisted of water being heated to 90 °C in a sealed container. Students were asked to describe what would be occurring at the macroscopic and molecular levels in these systems and to indicate what they could say about the rates of the processes occurring.

Pre-Test/Post-Test

The Conceptual Pre-Test on Solubility Equilibrium (CSPrT) was developed to evaluate student understanding of the dynamic nature of solubility equilibrium. The test was designed to discover misconceptions identified in the literature and in an earlier exploratory study. It is composed of 13 true/false and multiple choice questions and one short-answer question (*36*). The Conceptual Post-Test on Solubility Equilibrium (CSPoT) was identical to the pre-test. The test was reviewed by chemical education faculty members and graduate students and revised accordingly.

Worksheets

Two types of worksheets were given to the students to guide them toward the learning goals of the lesson, one providing more guidance than the other, as described in Akaygun and Jones (*44*) (Figures 3 and 4). An expert review of the content and the format of the worksheets was conducted by a science educator familiar with the simulation. The worksheets were modified on the basis of the review. The worksheets were also reviewed by chemical education faculty members and graduate students and revised accordingly.

2) Working with the animation
Watch the animation twice and observe what is happening. You can pause the animation at any time.
a) Fill in the given table for two different instances.

Cases		# Na^+ ions	# Cl^- ions	Saturated or not
1	dissolved			
	bound			
	total			
2	dissolved			
	bound			
	total			

b) Consider the case for a saturated solution. Now describe what you see and fill in the given table.
How do you know that the solution is saturated?

Cases		# Na^+ ions	# Cl^- ions	Saturated or not
1	dissolved			**Saturated**
	bound			
	total			

c) Were your predictions the same as what you observed? If not, how did they differ?

d) Was there a time when the saturated solution became unsaturated? If so, what happened to dissolve the salt?

e) When the solution is saturated the number of dissolved and bound ions fluctuates slightly. Why do you think this happens?

Figure 3. Sample questions from the more-guided version of the worksheet for the Table Salt portion of the lesson used by the Animation group.

Solubility is defined as grams of salt dissolved in100 mL of water (g salt/ 100 mL water).

Watch the animation twice and observe what is happening.

Design an experiment to calculate the solubility of table salt using the animation (or simulation).

Figure 4. Worksheet sample questions for the less-guided version of the same lesson as in Figure 3.

Attitude Survey

A five-question open-ended questionnaire was administered to measure student attitudes toward the lesson. The questions probed whether students found the lesson helpful, what aspects they liked and did not like, their suggestions for improving the lesson, and which part of the lesson they found most challenging.

Cognitive Load Survey

An eight-item questionnaire to measure cognitive load was prepared according to the guidelines of Brünken, Plass, and Leutner (*40*) and Paas and Van Merrienboer (*37*). Students were presented with eight statements and a nine-point Likert scale ranging from "very, very easy/low mental effort" to "very, very hard/high mental effort."

Data Analysis

The participant responses to the OCQ were coded according to the common features of the responses of the participants. A rubric was developed for this purpose. First, all the responses for a specific case were listed and coded. A rubric, the Mental Models of Equilibrium Scale (MMES), was developed to provide a different number (code) representing each different response (*36*). To assess the inter-rater reliability of the rubric, another chemical education graduate student rated 6 papers (19%). The evaluations of both scorers were compared and the rubric was revised. The initial agreement of the scorers before the revision of the rubric was 85% and the final agreement, in other words the inter-rater reliability, was calculated as 95% after the two raters rated a second set of papers using the revised rubric. For a more detailed explanation of the method of coding, see (*36*).

The responses of students to the Open-ended Conceptual Questionnaire (OCQ) were coded for two purposes: (1) to evaluate student understanding of

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these two equilibrium systems and (2) to determine the features emphasized in the students' mental models of liquid-vapor and solubility equilibrium before and after the implementation. These features were used as an indication of what the students thought was important in their explanations of the systems; the features can then be compared against the key features of expert mental models (*29*).

To address the first purpose of the OCQ, the Mental Models of Equilibrium Scale (MMES) was used to determine the mental models of experts and to identify the key features of expert mental models. This scale rates students' understanding of the dynamic nature of equilibrium on a scale from 1 to 5. Changes in students' understandings of solubility equilibria were assessed by comparing their initial and final scores on the same scale (Table 1).

Table 1. Rubric for evaluating mental models of solubility equilibrium

Scale	*Dissolving – recrystallization equilibrium*
5	Movement and 2 processes (dissolving & recrystallization)
4	Wrong terminology and 2 processes Movement and 1 process
3	Wrong terminology and 1 process Vague descriptions (e.g., interaction between intermolecular forces)
2	Movement statements only Only description of macroscopic/molecular features (I_2 and H_2O) Misconception about chemical reactions
1	Macroscopic statements Macroscopic and movement Structures only Unrelated concepts Chemical reactions and wrong terminology

A sample coding for a particulate level pictorial response to the OCQ is shown in Figure 5.

After coding students' responses on the Pre-OCQ, given before the implementation, and the Post-OCQ, given after the implementation, responses were coded with respect to the MMES. The Pre-OCQ and Post-OCQ were identical. Table 2 shows how the Pre-OCQ and Post-OCQ responses were coded according to the MMES.

To address the second purpose of the OCQ, the features of mental models that the students possessed before working with the computer visualization were tabulated and compared with the ones assessed after working with the computer visualizations using Chi-square analysis. The level of significance for determining the difference in features was taken to be 0.01 due to running multiple tests of independence during Chi-square analysis.

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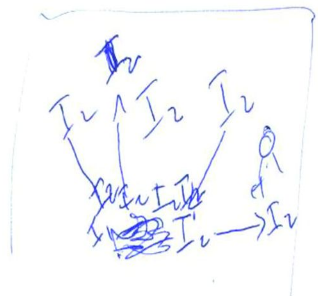
Student scores on the conceptual post-test (CSPoT) were compared by carrying out a one-way ANOVA. Perceived cognitive load was evaluated by assigning difficulty scores from 1 to 9 to student responses. Correlations between cognitive load scores and other measures were then sought. Student responses to the attitude questionnaire were coded and responses of the Animation and Simulation groups were compared by Chi-square analysis.



Flask: 0 (no representation of a flask)
Bottom of the flask: (no indication of bottom of the flask)
Solid: 1 (representation of solid/crystals)
Solution: 0 (no representation of solution)
Surface: 0 (no representation of surface)
Color: 0 (no representation of color)
Molecules: 1 (representation of molecules)
Structure: 1 (representation of structure with formula e.g. I_2, H_2O)
H_2O – I_2 Structures: 1 (indication of H_2O-I_2 positioning around)
Intermolecular interaction: 0 (no indication of H_2O & I_2 intermolecular interaction)
Saturation: 0 (no indication of saturation)
Dissolving: 0(no indication of dissolving)
Recrystallization: 0 (no indication of recrystallization)
Process: 0 (no indication of a process)
Dynamic nature: 0 (no indication of dynamic nature)
Equilibrium: 0 (no indication of equilibrium)
Motion: 0 (no representation of motion)
Rate: 0 (no indication of rate)
Misconception: 0 (no specific misconception)

Figure 5. A sample coding for a particulate level pictorial representation on the OCQ. The student was illustrating the processes occurring in a saturated solution of iodine in water at the molecular level.

Table 2. **Sample quotes of students describing the processes occurring in a saturated solution of iodine in water on the Pre-OCQ and Post-OCQ and their respective MMES scores.**

Pre-OCQ Quotes	*Post-OCQ Quotes*
"Molecules of water and iodine" *MMES=2*	*"Movement & recrystallization"* *MMES=4*
"All the iodine molecules mixed with water" *MMES=2*	*"Molecules joining and breaking apart."* *MMES=5*
"Movement and interaction" *MMES=2*	*"Salt ions and salt crystal"* *MMES=1*

Findings

Worksheets

Each student had been given one of two types of supportive worksheet to use while working with the simulation or animation. The worksheets differed in the amount of guidance they provided. No significant difference ($p > 0.01$) in any category, as identified in the OCQ, was discovered for groups using different worksheets but the same style of lesson. Therefore, for the data analysis participants were combined into the two groups Animation and Simulation, regardless of worksheet used.

Demographics

The majority of the college-level participants had familiarity with computer visualizations used in chemistry. Ninety-one percent said that they had seen science videos or animations before. Although 25% of the students did not indicate a specific topic for the video/animation viewed, 16% of the participants said the computer visualization they had seen was on molecular structure, 13% said it was on evaporation/condensation, 9% said it was on effects of temperature/pressure, 9% said it was on equilibrium, and the rest of the participants listed different topics such as interactions of atoms, protein denaturation, and hydrogen bonding. The majority of the students gave positive comments about the video or animation they had seen before. Sixty-six percent of the students said they thought it was helpful in understanding the concept and 16% said it helped them to visualize the phenomena at the molecular level. Only 3% said they thought it was not helpful.

Working with a simulation or animation was new to 50% of the high-school students. The other 50% stated that they had seen videos or animations on various topics such as bonding, relative sizes of atoms, energy levels and water. All the students who had seen a video or animation indicated that the lesson they had seen was helpful in understanding the concepts, providing a different perspective and helping them to visualize the material.

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Conceptual Pre- and Post-Test on Solubility Equilibria (CSPrT and CSPoT)

Students' understandings of dynamic solubility equilibria was measured by the conceptual pre- and post-test given before and after the implementation, respectively (see Appendix). Scores of each group on the pre- and post-test were compared by a paired sample t-test and no significant difference ($p > 0.05$) was found. In addition, no significant difference was found in the average scores of students in the combined groups on the conceptual pre- and post-tests, as shown in Table 3.

Table 3. Average scores on the CSPrT and CSPoT (maximum score = 25).

	Visualization	*N*	*Mean*	*Std. Dev.*	*t*	*df*	*Sig (2-tailed)*
CSPrT	Animation	21	16.00	4.056	.641	40	.741
	Simulation	21	15.10	4.647			
CSPoT	Animation	21	16.14	2.508	.000	40	.812
	Simulation	21	16.14	3.390			

One of the common misconceptions held by students was that all ions react with water during dissolving. In the analysis of the CSPrT, this misconception was seen in 84% of the students. After the implementation it decreased to 78%; however, the difference in these percentages was not significant ($p > 0.05$).

Changes in Mental Models of Solubility Equilibria

The students took the same Open-ended Conceptual Questionnaire (OCQ) before and after the implementation. Their responses to each question in the OCQ were coded with the MMES and analyzed by running a chi square analysis. The categories or key features representing mental models of physical equilibrium conditions were determined for both macroscopic and molecular levels (*36*). The mental models of students were compared separately: first for solubility equilibria, then for liquid-vapor equilibria, to check if they could transfer understanding to a different situation.

After the students' mental models were coded before and after the implementation, the Wilcoxon Signed Rank Test was run. Understandings of the dynamic nature of equilibrium for the combined groups before and after working with a computer visualization were found to be significantly different ($p < 0.05$). Average student scores for pre- and post-mental models are shown in Table 4.

Table 4. Average initial and final MMES score of students on understanding of dynamic solubility equilibria (Maximum score = 5).

	N	*Mean*	*Sig (2-tailed)*
Before treatment	42	2.33	.002
After treatment	42	3.29	

However, no significant difference in mean score was found between participants who had completed the simulation and those who had completed the animation. In addition, the post scores for the separate groups were not significantly higher ($p > 0.05$) than the pre scores. The comparison of both groups with respect to their initial scores on the assessment scale are shown in Table 5.

Table 5. Average MMES score of students in the two visualization groups on understanding of dynamic solubility equilibria.

	Visualization	*N*	*Mean*	*Sig (2-tailed)*
Before treatment	Animation	21	2.24	.226
	Simulation	21	2.43	
After treatment	Animation	21	3.19	
	Simulation	21	3.38	.907

Student mental models were characterized by identifying the features that appeared in student explanations. When the animation and simulation group were combined, changes were found in seven features of their mental models after the treatment: at the macroscopic level were macroscopic features, molecular features, solid, solution, structure, and process ($p < 0.01$). On the other hand, equilibrium was the only significantly different category found for the molecular level (that is, students were more likely to mention equilibrium after the lesson). Responses in no other categories changed significantly between the pre- and post- analysis. The changes in student mental models of solubility equilibria systems are summarized in Table 6.

It is interesting to note that, although the multiple choice test failed to reveal any impact of the simulation or animation on learning, analysis of the open-ended questionnaire did find an improvement in understanding of dynamic equilibrium. The features students chose to use in their explanations following the implementation of the simulation or animation were closer to key features that experts would use, suggesting that students had refined their mental models for the dynamic nature of equilibrium. New descriptions for the process features emerged, such as references to ions moving and recrystallizing. Examples of the responses for the molecular level given by of three students before and after the implementation are shown in Table 7.

Knowledge Transfer

The open-ended questionnaire that the students took before and after working with the solubility equilibria simulation or animation contained questions on two different physical equilibrium systems: liquid-vapor and solubility equilibria. In order to investigate whether the students could transfer their knowledge or understanding of dynamic nature from one equilibrium system to the other, students' understandings of the dynamic nature of equilibrium for the liquid-vapor system was assessed by coding the open-ended conceptual questionnaire. The average scores of the students in each group were compared on the MMES-LV (Mental Models of Equilibrium/Liquid-Vapor) scale before and after treatment by the Wilcoxon Signed Rank Test and no significant difference was found between the pre-and post assessment scores for the liquid-vapor equilibrium system. The results of the Wilcoxon Signed Rank Test are given in Table 8.

Although MMES-LV scores did not show an improvement, some differences in features appearing in the explanations were observed. Changes in the features students used in their explanations, which reveal their mental models of liquid-vapor equilibrium, were also analyzed by chi square analysis, but there was little indication of enhanced learning. For the macroscopic level five categories of features were found to appear in a significantly different number of explanations ($p < 0.01$) before and after the implementation. Following the visualization features that were mentioned more frequently were liquid water (from 4.8% to 14.3%), the presence of molecules (from 0 to 11.9%), and processes such as molecules entering or leaving the surface (from 0 to 7.1%). Features that were mentioned less frequently were the formation of steam (from 16.7% to 7.1%), presence of bubbles (from 23.8% to 16.7%), and macroscopic structures such as the flask (from 52.4% to 45.2%).

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Table 6. Significantly different features of the pre- and post-mental models of solubility equilibria systems expressed before and after treatment

Level	*Category*	*Pre-Mental Models*	*Post-Mental Models*
Macroscopic Level	Macroscopic features	21.1% solid at the bottom 14.3% solution & solid	31.0% solid at the bottom 23.8% solution & solid
	Molecular features	85.7% no molecular features 7.1% molecules dissolve	93.0% no molecular features 2.4% molecules dissolve
	Solid	38.1% at the bottom 2.4% solid dissolving	45.2% at the bottom 9.5% solid dissolving
	Solution	26.6% homogeneous mixture 2.4% saturated solution	14.3% homogeneous mixture 11.9% saturated solution
	Structure	26.2% iodine/I_2 2.4% macroscopic structure	16.7% iodine/I_2 14.3% macroscopic structure
	Process	16.7% dissolving 7.1% color change	9.5% dissolving 4.8% color change
Molecular Level	Molecular features	2.4% dissolving & recrystallizing 4.8% bouncing off	21.4% dissolving & recrystallizing 9.5% bouncing off
	Other processes	7.1% mixing together 0% ionization	0% mixing together 2.4% ionization

Table 7. Some student responses about the molecular level before and after the visualization

Before the visualization	*After the visualization*
Iodine dispersed	Some dissolving, some forming
Movement & interaction between water & iodine	Ions moving & recrystallizing
Few molecules	Ions moving around

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Table 8. Average score of students on the understanding of dynamic solubility equilibria in a new type of system

		N	*Mean of MMES-LV*	*Sig (2-tailed)*
Animation Group	– Before – After	21	2.57 3.10	.065
Simulation Group	– Before – After	21	2.62 2.43	.440

When the students' descriptions of the system at the molecular level were analyzed six categories of features were found to appear at significantly different frequencies before and after the implementation. Visualization features that were mentioned less frequently were the rates of processes (from 54.8% to 35.7%), evaporation (from 64.3% to 52.4%), and condensation (from 28.6% to 19.0%). Features that were mentioned more frequently were equilibrium (from 21.4% to 23.8%) and an indication that molecules split when evaporating (from 2.4% to 9.5%). It can be seen that when explaining events at the molecular level the students mentioned molecular properties more frequently, while references to macroscopic features decreased significantly.

No significant differences in the pre- and post- analysis were found for any other category. In addition, there was no difference in the MMES scores of students in the Animation and Simulation groups.

An interesting finding was that after viewing the simulation or animation of solubility equilibria, students tended to explain the liquid-vapor equilibrium system by referring to the solubility system, even by using solubility concepts such as ions splitting apart and merging with the solute.

Cognitive Load Questionnaire

When the scores on the cognitive load questionnaire for the students who worked with animation and simulations were compared by an independent samples t-test, no significant difference ($p > 0.05$) was found between the groups (Table 9).

Correlations were sought between the perceived cognitive load of the computer visualization (PCLV) with post-mental model scores (MMSE-Post) and conceptual post-test scores (CSPoT) for the combined groups. The correlations for the given tests are summarized in Table 10. No correlation with post-mental model score was found. However, the correlation between the perceived cognitive load of visualization (PCLV) and the conceptual post-test on solubility equilibria (CSPoT) was found to be significant and negative. This result suggests that students who perceived the visualization as having high cognitive load scored low on the conceptual post-test. The lack of correlation with the MMSE-Post score may indicate either that students did not find the open-ended OCQ questions to be as challenging as the multiple-choice and true/false questions of the CSPoT or that the OCQ questions were more closely related to the simulation and animation.

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Table 9. Comparison of Perceived Cognitive Load of Visualization (PCLV) for the students in the animation and simulation groups.

Perceived Cognitive Load of the Visualization (PCLV)	*N*	*Mean*	*t*	*Sig. (2-tailed)*
Animation	21	4.58	0.173	0.134
Simulation	21	4.51		

Table 10. Correlations between perceived cognitive load and test scores for the combined groups

Tests	*N*	*Pearson Correlation*	*Sig. (2-tailed)*
PCLV & MMES-Post	42	.108	.495
PCLV & CSPoT	42	-.408[a]	.007

[a] Correlation is significant at the 0.01 level (2-tailed).

Attitude Questionnaire

The responses of the students to the five questions on the attitude questionnaire were coded and a frequency analysis was performed. The results for the combined groups are summarized in Table 11.

The chi-square analysis for the attitudes of the participants showed that there was no significant difference ($p > 0.01$) between the Animation and Simulation groups on the evaluation of the lesson as helpful or not. Similarly, no significant difference was found between the groups in terms of how positive they were about the aspects liked or disliked, the parts found challenging, or suggestions coming from the students. Some of the students in each group indicated that they liked to see the dissociation and recrystallization of the salts; that is, the dynamic nature of the equilibrium system. In addition, when the aspects liked and disliked were compared within the groups who viewed a simulation and an animation, it was observed that 44% of the students who used the animation expressed a desire to control the variables themselves, that is, they wanted to use a simulation instead of an animation.

The attitudes of participants towards the computer lesson are summarized in Table 12. The majority of the students in both the Animation and Simulation groups said that the computer lesson was helpful. Only two students in each group did not find the computer lesson helpful.

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Table 11. Frequency analysis for the attitude questionnaire

Category	*Subcategory*	*N*	*Percent (%)*
Helpful or not	Not helpful	4	10
	Partially helpful	10	24
	Helpful	28	67
Aspects liked	Helpful in visualizations	10	24
	Helpful in conceptual understanding	5	12
	Particular features of the simulation	1	3
	Interactivity	9	21
	Simplicity	6	14
	Enjoyable	3	7
	Dynamic nature (equilibrium & motion)	3	7
	Ability to make comparisons	3	7
	No aspect	2	5
Aspects disliked	Worksheet questions	11	26
	Lack of explanations	4	10
	No interactivity	3	7
	Length of the lesson	1	3
	Complexity	10	24
	Particular features of the simulation	1	3
	Graphics	1	3
	Technical problems	5	12
	Boring	2	5
	No aspect	4	10
Suggestions about	Simulation	13	31
	Worksheets	8	19
	Lesson	17	40
	No suggestion	4	10
Challenging Part	Table salt	4	10
	Slightly soluble salts	9	21
	Design a salt	20	48
	Slightly soluble salts & Design a salt	3	7
	Table salt & Design a salt	1	2
	The math	1	2
	No challenging part	4	10

Typical student quotes are shown in Table 13. The reasons given by the students for finding the lesson helpful were found to be similar for each group. Four students in the Animation group and six students in the Simulation group said that the simulation or animation helped them to visualize the solution system. The larger number of students mentioning the visualization in the Simulation group might be related to the fact that these students were able to explore the simulation. Seven students in the Animation Group and six students in the Simulation Group said they liked the visual aspect of the simulation or animation. In addition, six of the students who worked with the simulation said they liked the interactivity and having the power to change the variables.

Table 12. Attitudes of students in different groups towards the computer lesson

Group	*N*	*Helpfulness*	*Number*
Animation	21	Not helpful	2
		Partially helpful	2
		Helpful	17
Simulation	21	Not helpful	2
		Partially helpful	8
		Helpful	11

Table 13. Sample student quotes showing the attitudes towards the computer lesson

Item	*Student Quote*
Helpfulness	Animation: *"No, it confused me more, no instruction provided"* *"Yes, it allows a student to visualize what's really going on"* Simulation: *"Yes. Able to visually observe what was going on in solution with asalt and the solubility process"* *"Yes, it helped me to visualize the reactions"*
Aspects liked	Animation: *"The pace and visuals"* *"The demonstrations of different salts being added to water"* Simulation: *"Could make own salts, add more or less salt, change the charges, and change K_{sp}"* *"I liked the visual and that I could visually see what was going on"*
Aspects disliked	Animation: *"It was long"* *"Hard to understand"* Simulation: *"The math to calculate K_{sp}"* *"I did not like the questions. Sometimes they were confusing"*
Suggestions	Animation: *"I think I would have liked doing it myself instead of just watching the animation"* *"Have an intro"* Simulation: *"Have a 'text' lesson followed by further explanation using video & pictures"* *"More directions/guidance"*

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The aspects disliked by the students showed similarities and differences for certain categories. Two students in the Animation Group said that they did not like the lack of narration. This feeling might have arisen because they needed to have additional information or explanation. Five students who worked with the animation said that they did not like not having the power to change the variables. Two students from each group said that the visualization they worked with was not easy to understand. The suggestions of students for the improvement of the study varied. Two students in the Animation Group and one from the Simulation Group said that they wanted to work on more and different simulations. Four students in the Animation Group suggested including more interactivity in the animations. Three students in the Animation Group and six students in the Simulation Group suggested including more explanations or directions on the worksheets. The larger number of students in the Simulation Group requesting more information may be a result of the fact that these students had to make many decisions about how to proceed through the lesson. When the students were asked to name the most challenging part of the simulation or animation, the listings were similar between the groups. Eleven students in the Animation Group and nine students in the Simulation Group agreed that a specific section, 'design a salt' that required deeper conceptual understanding, was the most challenging.

The attitudes of students for the aspects discussed above did not show significant differences ($p > 0.05$) when they were compared by a chi-square analysis with respect to gender, career goal, computer visualization experience, and course grade expectation. Having previous computer visualization experience might have had an effect on the attitudes of students towards the helpfulness of the computer lesson because only one student out of 34 who said they had prior experience but three out of eight who said they did not have previous computer experience found the simulation or animation not helpful. This difference was found to be significant ($p = 0.009$).

Interviews

Two volunteer interviewees from each treatment group, four in total, were selected and interviewed with a think aloud protocol. Summaries of their comments are reported here, followed by a table summarizing comments made by two or more of the four students.

The interviewees described how they worked through the simulation or animation of solubility equilibria and answered questions about the positive and negative aspects of the visualization and their suggestions for the improvement of the visualization. The key features of the visualizations determined by the participants are described in Tables 14-17.

Table 14. The aspects emphasized by Participant 4 (Simulation Group, worksheet with more guidance) during the interviews

Categories	*Aspects emphasized*
New knowledge gained	- saturation by seeing the crystals forming - formation of precipitates on the sides of the beaker - dissolving and recrystallization (it doesn't stay constant) - comparison of solubilities (one salt is more soluble than the other) - the effect of charges and K_{sp} on solubility - drew a representation of a generic salt
Positive Aspects	- ion counter showing number of ions dissolving and precipitating. - visualizing the saturation - being able to design own salt. - interactivity
Negative Aspects	- none
Suggestions	- use other solvents (acid or base) - being able to change temperatures

Table 15. The aspects emphasized by Participant 6 (Simulation Group, worksheet with less guidance) during the interviews

Categories	*Aspects emphasized*
New knowledge gained	- how salt dissolves in water - how much water is needed to dissolve the salt completely - comparison of solubility (time to dissolve) of different salts - the effect of K_{sp} on solubility - the interaction between each molecule/ion is different - how K_{sp} is related to different kinds of salts. - attaching and breaking of ions - drew a representation of a generic salt
Positive Aspects	- colors coding of the ions - showing different charges and how different salts act differently. - visual representation
Negative Aspects	- hard to associate K_{sp} to solubility - worksheet was hard.
Suggestions	- more instructions on how to use - addition of narration

Table 16. The aspects emphasized by Participant 5 (Animation Group, worksheet with more guidance) during the interviews

Categories	*Aspects emphasized*
New knowledge gained	- how the sodium and chloride ions react in water - comparison of solubilities (time to dissolve) - solubility depends on the charges - the concepts in 'design a salt' are difficult to understand - drew a representation of table salt
Positive Aspects	- showed variables - showed more of an image of something that can't be actually seen. - visual representation - animations made the concepts easier.
Negative Aspects	- a lot of information being shown on the side, which is a little harder to get. - concepts are difficult.
Suggestions	- addition of narration - addition of an explanatory text

The aspects emphasized by two or more participant interviewees are summarized in Table 18.

The interviewees from both groups appeared to feel that they had gained a good understanding of dissolving of a salt, comparison of solubilities of different salts, saturation, effect of charges and K_{sp} on solubility, dissolving and recrystallization, and formation of crystals on the sides of the container, after working with the solubility equilibrium simulation or animation.

The main positive aspects of the visualizations mentioned by the participants were the visual representation, ion counter, and the helpfulness of the visualizations to conceptual understanding. Negative aspects were primarily related to the graphics of the animation, because the interviewees who worked with an animation said they were not able to read the ion counter easily. Due to the fact that the animation was a screen-captured version of the simulation, the resolution of the video may not have been as high as in the case of the Java simulation. Moreover, the students who worked with the simulation had a chance to work at their own pace and so they could pay more attention to the changes occurring, including the ion counter. The suggestions made by the interviewees mainly included adding explanatory audio or text, because they said they felt more instructions needed to be given.

Four experts, two university instructors and two high school chemistry teachers, were interviewed. One expert from each category viewed the simulation and the other viewed the animation during the interviews. The experts who viewed the animation had also seen the simulation. Each expert was asked to evaluate the computer visuals in terms of strengths, weaknesses and their suggestions for improvement. The aspects emphasized by two or more of the experts are shown in Table 19.

Table 17. The aspects emphasized by Participant 7 (Animation Group, worksheet with less guidance) during the interviews

Categories	*Aspects emphasized*
New knowledge gained	- saturation is the maximum amount that will dissociate in water, when you see precipitate they won't dissociate in water. - as salt is added to water, Na and Cl molecules dissociate in water. - didn't understand why the number of ions on the counter are fluctuating. - didn't understand what made the salt more or less soluble. - as K_{sp} got higher (less negative), the salt was more soluble - drew a representation of K_{sp}
Positive Aspects	- the numbers on the counter helped to see what was happening (for example, the effect of K_{sp} on solubility when the other variables are held constant. - the visual representation
Negative Aspects	- hard to see the correlation between the numbers on the counter and the animation. - hard to understand the effect of K_{sp} - no narration - hard to catch that the numbers were changing at first.
Suggestions	- addition of narration - addition of an explanatory text - prefers simulation and having the power of controlling the variables - making a notice for the number to be changing - prefers a more guided worksheet.

As summarized in Table 19, all the experts agreed that the solubility equilibria visualizations demonstrated well the concepts of dissolving of a salt and saturation, dynamic equilibrium and random motion. Interactivity and the ion counter appear to be the other powerful aspects of the solubility visualizations. However the movement of the ions towards the drain (an artifact of the software program) and the use of a beaker with an inconceivably small volume were the weaker aspects, because it was thought that they might mislead students. In order to improve the effectiveness of the visualizations, the experts suggested adding explanatory text or instructors' notes, including conceptual questions, and using a legend for the ions.

To obtain expert opinions on the effectiveness of the simulation and the animation, two experts who had already used the simulation were interviewed while they were using the animation. One of the experts felt that the animation was equivalent to the simulation in terms of displaying the motion of ions and the dynamic equilibrium, whereas the other expert who viewed the animation preferred using the simulation to the animation because of the ability to change the variables, which may help students learn by increasing their curiosity.

Table 18. Aspects emphasized by two or more of the four interviewees

Categories	*Aspects emphasized*	*Number of participants*
New knowledge gained	- Dissolving of salt	4
	- Comparison of solubilities	4
	- Saturation	3
	- Effect of charges and K_{sp} on solubility	3
	- Formation of precipitates on the sides of	3
	the beaker	2
	- Dissolving and recrystallization	3
	- Representation drawn	2
	table salt	
	design a salt	
Positive Aspects	- Visual representation	4
	- Ion counter	2
	- Helped conceptual understanding	2
Negative Aspects	- Conceptual difficulty	2
Suggestions	- Add narration	3
	- Add an explanatory text	3

Table 19. Aspects emphasized by two or more of the four expert interviewees

Categories	*Aspects emphasized*	*Number of experts*
Strengths	- Demonstration of dissolving of a salt and	4
	saturation	4
	- Demonstration of dynamic equilibrium	4
	- Demonstration of random motion	3
	- Scientifically accurate	2
	- Interactivity	2
	- Ion counter	
Weaknesses	- Movement of the ions towards the drain	2
	- Small amount of volume shown	2
Suggestions	- Add an explanatory text or instructors' notes	3
	- Use a legend for the ions	2

Limitations

The worksheets themselves provided an interactive environment, even for the animation, reducing the difference between the learning environments experienced by the two groups. The guidance provided by the worksheets may have distracted students in the simulation group from interacting with the simulation in the free exploration mode its developers recommend (*56*). The worksheets may also have minimized the differences between the treatment groups by focusing attention on target concepts.

Conclusions

The results show that significant changes in student mental models of solubility equilibria at both macroscopic and molecular levels occurred after completing the simulation or animation. When describing the macroscopic level of the solubility equilibrium system, the percentage of students who mentioned key macroscopic features such as solid and solution increased significantly. In addition, the percentage of students who mentioned molecular features such as the term 'molecules', iodine and dissolving while describing the macroscopic level decreased significantly. In other words, students were more likely to use macroscopic features and less likely to use molecular features for the macroscopic level, suggesting that they may have been distinguishing the two levels more clearly. For the molecular level, significant increases were observed in the percentage of students mentioning dissolving and recrystallization, and molecular features, such as molecules bouncing off one another. However, one of the students incorrectly mentioned ionization, even though no student had mentioned ionization prior to the lesson. This error might be considered an effect of the computer visualization on students' understanding since the visualization showed salts dissociating into separate ions when dissolving.

The ability of students to transfer their understanding of dynamic equilibrium from one equilibrium case to another was assessed by investigating the changes in mental models of liquid-vapor equilibrium as measured by the OCQ. When the changes of student mental models of the liquid-vapor equilibrium system were analyzed by chi square analysis, the results suggested that there were significant changes in the key features of the mental models for both macroscopic and molecular levels, but these changes did not imply enhanced learning. At the macroscopic level the percentage of students mentioning macroscopic features such as vapor/steam/bubble, bubbling, and macroscopic structures decreased significantly. In addition, the percentage of students who said 'molecules split' on evaporating increased significantly, possibly due to the fact that in the computer visualization of solubility ionic compounds were shown separating into individual ions as they entered the water. In other words, students transferred knowledge from the visualization to another situation inappropriately.

In this study it was found that an open-ended test in which responses can be coded to identify features of explanations was more effective than a multiple choice test when measuring changes in mental models. Although comparison of the scores on the conceptual pre- (CSPrT) and post- (CSPoT) test on solubility equilibria revealed no significant change, changes were seen in student mental models when an open-ended instrument was used. When the students' mental models of equilibrium were assessed for the solubility equilibrium system by the MMES, a significant increase in their understanding of the dynamic nature of solubility equilibrium was observed when the groups were combined. The computer visualization, whether animation or simulation, had a positive effect on their understanding of solubility equilibria.

Students' mental models of equilibrium were also assessed for the liquid-vapor equilibrium system by the MMES to assess transfer of understanding to a different equilibrium situation. The results of the analysis showed that there was no significant difference in their understanding of the dynamic nature of liquid-vapor equilibrium. Little impact of the computer lesson on solubility equilibrium on their understanding of liquid-vapor equilibrium was observed, suggesting that it was difficult for students to transfer their knowledge to a new situation. Because these results differ from the finding of Mayer and Chandler (*23*) that learning from a simulation enhances transfer to new situations, it may be that the liquid-vapor system was so different conceptually that transfer was not easily made.

When students who had worked with the animation were compared with students who had worked with the simulation, it was found that both groups of students had better conceptual understanding of the dynamic nature of equilibrium. Being able to control the variables in a simulation did not create a significant difference in learning in this study over not being able to control them. This result differs from an experiment in which computer simulations were compared with instructor demonstrations in a physics class (*57*). In that case the students completing the simulations scored higher than the students who viewed the demonstration on three of four topics. In this case the simulation was compared against an animation that presented the same information, but without control of the variables. There may be two explanations for the lack of difference in achievement in this study. First, the visual representation of a solution at the molecular level might have been the most important factor in helping students to visualize what is happening in solubility equilibria. Therefore, it did not matter whether they manipulated the variables or the variables were manipulated for them. Second, although students could control variables in this simulation and view the effect of their choices, this specific simulation did not provide feedback on understanding and that degree of interaction may not have been enough to create a significant effect on students' understanding.

Neither animation nor simulation was perceived to require a high cognitive load and students had positive attitudes toward both types of lesson. However, students who had worked with the animation expressed a desire to control the variables.

Interviews with students revealed some difficulties students had with the simulation and animation. The students suggested adding more information on the content of the lesson. Interviews with instructors revealed that the lessons were well received by the instructors and that instructors would appreciate having some instructor guidelines for the use of the lessons. Such guidelines are available on the PhET web site (http://phet.colorado.edu/).

Implications for the Classroom

The results of this study suggest that simulations and animations can both be used to enhance learning in chemistry classes with guidance such as that provided by the worksheets. However, a concern with classroom usage of animations is that students in the Animation group of this study were able to control the pacing, something that might be difficult to achieve in a lecture hall. In addition, independent exploration may have other advantages not investigated in this study. It has been reported that when students have the opportunity to explore the PhET simulations on their own they may pose their own questions and attempt to use

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the simulations to answer their questions in a manner similar to that used by professional scientists (*56*). In such a learning environment students can build inquiry skills and expand their knowledge in different ways. The optimal use of interactive simulations might include both lecture presentation and independent student usage, so that students are provided with the orientation required to use the simulation well, yet have the opportunity to explore it on their own (*54*).

Implications for Research

These results suggest that coding student responses to open-ended questions may be necessary to detect changes in student mental models of chemical systems. In future research the use of the simulation and animation without the support of worksheets, a more challenging learning environment, should be explored. It has been shown that students gain more from simulations of physics concepts when appropriate scaffolding is used to engage their attention and interaction (*58*). The degree and type of scaffolding required for chemistry simulations should also be studied.

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Appendix

Code:

Solubility Equilibria Post Test (CSPoT)

(Same as Pre Test, but with content rearranged)

1) Circle True or False for each of the following explanations of what happens when a salt dissolves in water. For "False" statements only, briefly explain the reason for your answer.,

True / False: The ions in a crystal dissolve mainly from the <u>top</u> (upper side) of the crystal.

True / False: The ions dissolved in the solution are in constant motion.

True / False: When a salt dissolves in water or another solvent, there is a

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chemical reaction between the salt and the water or solvent.

True / False: In a saturated solution of a salt, there are always some ions in thesolid dissolving and some ions in solution crystallizing.

2) Select the correct statement for a saturated solution of a salt in water that has some precipitate at the bottom of the flask.

a) All the ions are bound in the solid crystal.

b) All the ions are dissolved in the solution.

c) Some ions are in the solid and some are in the solution.

3) Which one of these factors causes the ions of a salt to dissolve in water?

a) Attractions between water molecules and the ions of the salt.

b) Repulsions between water molecules and the ions of the salt..

c) Repulsion between ions having the same charges (anion – anion and cation – cation).

d) Attractions between oppositely charged ions (anion – cation).

4) Which one of the following statements is true for the precipitation of AgCl?

a) Ag^+ and Cl^- ions first pair up in the solution, then the pair sticks to the crystal.

b) Ag^+ and Cl^- ions stick to the crystal independently.

c) First all the Ag^+ ions stick to the crystal, and then the Cl^- ions stick.

d) First all the Cl^- ions stick to the crystal, and then the Ag^+ ions stick.

For items 5-14, mark each T (true) or F (false):

5) In a saturated solution, the concentration of dissolved ions constantly decreases.

6) Solubility depends only on K_{sp}, not on the formula of the salt.

7) Of the slightly soluble salts AX and BY, the one with a K_{sp} value having the more negative power of ten will precipitate first.

8) When the K_{sp} values of two salts having the generic formulas AX and B_2Y_3 are the same, their solubilities will be the same.

9) When a solution of a salt is saturated, no crystals grow on the sides of the container, they only deposit on the crystal at the bottom of the container.

10) When you add water to a saturated solution, you will be able to dissolve more salt because its concentration has decreased.

11) A saturated solution is a dynamic system in which ions can collide with each other

12) When ionic solids dissolve in water, spheres of hydrations form around cations and anions.

13) When a solution becomes saturated, the ions in solution are in equilibrium with the ions in the crystal.

14) Write a balanced chemical equation for dissolving of PbI_2

15) Circle the numbers of the questions that the simulation helped you answer.

1 2 3 4 5 6 7 8 9 10 11 12 13 14

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Chapter 7

Virtual Worlds and Their Uses in Chemical Education

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Virtual worlds have a unique capacity to immerse the user in an online community. This experience is helping students learn many subjects, including chemistry. This chapter introduces virtual worlds with special attention paid to *Second Life*, the most popular virtual world used in education. The next chapter section explains various efforts by educators to enhance their courses with *Second Life* and the benefits of doing so. The author then describes why virtual laboratory experiments are well-suited for college chemistry courses and presents preliminary results of a study in which chemistry students performed an experiment in *Second Life*.

Introduction to Virtual Worlds

Technology allows us to create and join a wide variety of virtual worlds through computer games and simulations. As with books, all video games attempt to a certain extent to create an alternate reality for the people to temporarily immerse themselves. In some games, such as those in the *Myst* series, a single player solves complex puzzles in richly detailed fantasy worlds. Other games require players to compete or collaborate with each other online and in real time. *World of Warcraft* and *Second Life* (SL) are examples of this later type of virtual world and are referred to as massively multiplayer online games (MMOGs) because of the large number of simultaneous participants. This type of game evolved from text-based MUD (multi-user dungeons) in the 1980s (*1*). Over time, designers have improved many aspects of virtual worlds, including: visual and auditory details of three dimensional surroundings, ability to interact with objects

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and other participants in the virtual environment, freedom of movement and actions, and the accuracy of physical laws, such as conservation of momentum (*2*). Virtual worlds in modern MMOGs incorporate all of these features. Users observe their virtual representations, known as avatars, within a virtual world shared with by other avatars. They communicate with each other through text, gestures and speech over the internet. Through their avatars, users share, trade and purchase items, establishing an economy within the virtual world itself. Some virtual worlds allow users to create objects within the game as well. The narrative of a MMOG, if one exists at all, is loose and open-ended. Social interactions that players experience within the game largely determine the degree to which they feel immersed in the virtual environment (*3*).

Video gaming in general has become a major source of consumer entertainment. Their gross sales revenue in the United States totaled over $16 billion in 2011. This includes games played on consoles, computers and hand-held devices (*4*). To put the importance of video games in perspective, consider that combined movie box office (*5*) and DVD sales (*6*) in the US were about $12.5 billion during the same year. Games such as *Assassin's Creed* and *Call of Duty*, although not MMOGs, are among the most popular video games because players feel immersed within the games' realistic virtual environments. Virtual worlds within computer games are entertaining and profitable.

Virtual worlds such as *World of Warcraft* have objectives or quests for avatars to accomplish. Completing tasks is necessary for achieving benchmarks within the game and participating in the game's fantasy narrative. As avatars reach these goals, they gain new abilities and wealth, allowing them to attempt more difficult quests. Players themselves gain experience playing the game and social status within the gaming community based on their accomplishments. In many cases, combat is a primary activity. Developers of online games such as *Unreal Tournament* and *Neverwinter Nights* permit users to modify their games in many ways, allowing educators to change the game's objective from slaying an enemy to answering a quiz (*7–9*). However, these modified games can still retain violent characteristics. For this reason, some educators criticize these educational games despite their adaptations due to the preceived lack of appeal towards female students. This criticism is based on the evidence that female students prefer collaborative, rather than competitive, learning experiences (*10*). Although combat has a central role in many of these computer games, diplomacy, problem solving and teamwork are important as well. Players work together because many quests require elaborate team strategies to defeat an enemy. Mentoring takes place in clans, teams and guilds within the fantasy world.

Second Life, *The Sims* and similar games place a greater emphasis on building relationships among players through interactions of their avatars. Violence and aggression are discouraged or simply not allowed. In fact, an avatar cannot "die" in *Second Life* and avatars in *The Sims* can die only through various nonviolent means. (Second Life does allow users to play combat-oriented role playing games in which avatars can be hurt. However, the avatar's wounds are not permanent.) These games lack an overarching storyline and allow for indefinite play. In particular, the game design of *Second Life* encourages its players, known as residents, to explore the virtual world with their avatars, build or create content within the virtual world and interact with other avatars. There is no SL scoring system or levels of advancement – residents continue to enter SL in order to meet each other, participate in the virtual economy and visit new places. While these activities seem mundane compared to vanquishing dragons and evil sorcerers, playing *Second Life* can provide residents with the same rich and meaningful experiences which they enjoy in real life. Emphasizing users' experience in gaming environment itself leads some to refer to *Second Life* as a multi-user virtual environment (MUVE), as a way of distinguishing it from a more goal-oriented MMOG.

Finding a Second Life

Phillip Rosedale founded Linden Labs in 1999 with the purpose of creating a virtual world to bring people together within an online community. The San Francisco technology company launched *Second Life* in 2003 (*11*). The number of SL residents increased quickly starting in 2007 after SL received significant coverage in the press and popular culture. For example, the popular detective show NCIS featured a criminal investigation involving avatars in *Second Life* (*12*). At its peak, an average of 65,000 residents were logged in at the same time in 2009. This number declined but reached a steady value of 50,000 concurrent users in 2011 (*13*). Over 1 million users log in at least once each month and this population has grown slowly since 2009 (*14*). Other virtual worlds exist but *Second Life* is the one most widely known by general public and among educators.

Setting up an SL account is straightforward and necessary for becoming a resident. Since Linden Labs occasionally modifies its account procedures, readers are encouraged to view the current system requirements and rules (*15*). In general, a user selects an avatar appearance (which can be changed later), provides an email address and creates a username and password. A user must then download the client software, known as the *Second Life* Viewer, in order to log in. A user interacts with the virtual world through the keyboard, microphone and mouse.

There are a few potential barriers to entry for new residents. Most importantly, *Second Life* is graphics-intensive so residents may experience problems using older computers. A broadband connection, preferably wired, is also necessary. Teens as young as 16 years old can enter SL with restrictions on their exposure to adult-themed areas. Younger teens receive access with greater restrictions. This policy may prevent educators in middle and high school from taking full advantage of *Second Life* for their classes but it should not pose problems for college faculty. Cost does not limit access to SL because a basic account is free and provides full access. Most residents choose a basic account. Its only noteworthy limitation is that residents with a basic account cannot purchase land. For that, a premium account with a current cost of $72 per year is necessary. A premium account also entitles the resident to higher quality technical support and a monthly stipend of Linden Dollars, the SL currency.

The SL Mainland consists of many continents designed by Linden Labs. Private estates are regions located beyond the Mainland and are created by residents. Since these regions are surrounded by water, they are referred to as islands. Space on the Mainland is finite but there is no limit to the number of private estates. If a resident buys an island, Linden Labs simply creates one and deletes it if the account is closed. Regions have a geographic location within *Second Life* but that is somewhat inconsequential since avatars can teleport to any specific location they desire (*11*). In total, the virtual landscape spans approximately 2000 square kilometers, the same area as the city of Jacksonville, Florida (*14*).

Many colleges, universities and individual faculty members own SL land in order to host virtual campuses, classrooms and areas for conducting research and meetings. Land owners can set access restrictions to allow or ban certain individuals or make the area open to everybody. An educator does not need to own land for students to learn in *Second Life* since there is already much SL educational content available. This situation is analogous to the world wide web - an educator can create a website to post educational content or link to websites owned by others. Relying on other people's websites is easier but their accuracy and continuous availability are always in question. Often, educators are willing to share their land with colleagues who need a small, temporary space to teach.

Before jumping into *Second Life*, educators should know that the learning curve is steep, though tutorials are available online. Students will experience challenges initially though they might view them in a positive light (*16*). Entering a strange and new virtual world can be overwhelming and training is essential (*17–22*). Educators can create tutorials that feature videos available on YouTube to help students adjust to their new environment. Students can accomplish the simplest of tasks on their own. Building objects and other complicated procedures can be covered in small group tutoring sessions either in a real classroom or in *Second Life* itself (*20*).

The most distressing technical problem for faculty is that Linden Labs occasionally requires updates for the SL Viewer to correct critical errors. This leads to two problems. First, the update can interrupt class. Second, computer security settings on school-owned computers can require IT personnel to perform software updates. Students would have to perform their work in SL later, outside of class. If students use their own computers, the instructor should clearly explain the computer system requirements and show them how to determine if a computer can operate the SL Viewer (*17*). Accessing *Second Life* from a school network can be a challenge because some firewall settings might prevent students from logging in (*23*). Planning ahead and working closely with the IT department is wise.

Griefing is harassment and deviant behavior by avatars. Even though the victim of griefing doesn't suffer any physical damage, encounters with griefers can be disturbing. Griefing takes many forms, including vulgar language and gestures, overloading the SL Viewer software or pushing an avatar (*24*). None of these methods of griefing cause permanent damage, though having to restart the SL Viewer does shift the harassment from the purely virtual world at least partially into the real world. Griefing can and has disrupted business (*25*, *26*) and the learning experience of real students and instructors (*27*). Though it can be common (*28*), land-owning educators can grant access to a space only to students' avatars and nobody else. This strategy can prevent avatars from interferring with class.

Second Life is very different from reality in certain ways. Game designers make some affordances so that residents avoid the most boring or undesirable aspects of real life. Avatars can teleport or fly instead of walking. They do not have to eat, address hygiene needs, exercise or sleep. Avatars do not age. Residents may elect that their avatars perform these actions. For instance, a player may wish her avatar to eat at a cafe as part of a desire for social interactions. Since avatars do not need to meet their basic physical needs, avatars do not need jobs. Avatars can acquire and carry an unlimited number of items without concern for their weight or size. Other SL game features allow players to express themselves more easily than in real life. A resident can customize his or her avatar's appearance at any time, including hair, muscularity and any other physical feature, even those beyond a human form (Figure 1). Avatars augment their typed or spoken words with appropriate gestures, in the same way that people speak in the real world.

Figure 1. Winkelmann Teichmann, the avatar of the author, Kurt Winkelmann.

Second Life has a thriving economy with shopping as the most common economic activity. Residents create items and sell many items, including cars, houses, pets, clothes and newspapers. Transactions between residents in different countries are possible because there is a common virtual currency. The Linden Dollar (L$) is the unit of SL currency which residents can exchange for real world currency. The SL economy functions successfully with little outside interference from Linden Labs and with a strong respect for property rights of land owners and content creators. Linden Labs does not claim rights to its users' created content or their intellectual property (*29*). Why would anybody spend real money on virtual items for an avatar? Residents feel their avatars are an extension or reflection of themselves so they want them to look good and fit in with community members.

Just like in real life, creating a virtual device is more challenging than buying or using it. Residents can easily create a simple item, such as a sphere or cube, using the editor found in the *Second Life* Viewer. This is known as building a primitive object (prim). By themselves, prims do nothing but they become active when a resident adds programming commands, known as scripts. Scripts instruct the prim when and how to respond to an event. For instance, a prim in the shape of a lantern might light itself when an avatar touches it. Scripts are written using Linden Scripting Language (LSL), a language unique to *Second Life* but similar to the programming languages C and Java. As with other aspects of *Second Life*, many tutorials and groups exist to help residents learn to script (*30*).

Learning in *Second Life*

The role of *Second Life* in higher education is growing. Initially, schools established SL campuses as a way to advertise and recruit students (*31*). Researchers attend conferences in *Second Life*, saving time and money otherwise spent traveling (*32*, *33*). Most importantly, educators are now conducting SL-based classes in a variety of disciplines. Though not intended as an exhaustive list, college-level disciplines taught in SL include archeology (*20*, *35*), biology (*36*), computer science (*21*, *37*), education (*17*), engineering (*38*, *39*), English (*17*, *18*), Library studies (*40*), information systems (*41*), media and communications (*17*, *20*, *35*, *42*), medicine and health (*43–47*), photography (*20*, *35*), physics (*48*, *49*), psychology and psychiatry (*19*, *50*, *51*), and security (*52*, *53*). A review of recent peer-reviewed education journals shows that the field of medicine, particularly nursing, is taking most advantage of *Second Life* as a venue for teaching. Virtual worlds provide professional development for K-12 educators (*34*). Education for K-12 students is limited by Linden Lab's restrictions on the ways that avatars of adults and minors could interact.

Chemical educators are active in Second Life also. Bradley and Lang present many examples of how SL can help faculty teach chemistry in their review article - the first presentation of chemistry in Second Life to appear within an academic journal (*54*). Students build large molecular models then rotate them, zoom in and even see how they react. Proteins in Second Life can show different chemical features by highlighting certain amino acids or mapping polarity. A script imports data for such complex structures from open source chemical databases. Second Life can also show the shapes and geometries of atomic orbitals (*22*, *55*). Dr. Wendy Keeney-Kennicutt of Texas A&M University presents her study of how students learn about molecular shapes and Valence Shell Electron Pair Repulsion (VSEPR) theory in Second Life in the next chapter of this book. Professor Jean-Claude Bradley created a chemical spectrum game in Second Life in which students interpret ^{1}H NMR and other spectra for the identification of unknown compounds. The spectra are taken from real data sources so the spectra include solvent peaks and peak imperfections. Such features allow students to practice interpreting real spectra (*56*). Educators find virtual worlds useful in a number of ways, including improvement in both student academic performance and attitudes about the course. Some students are more comfortable within a virtual world compared to other ways of attending class – a welcome break from sitting in a lecture hall (*57*). Given the apprehension of working with chemicals (*58*), this benefit might be generalized to laboratory settings as well. Students in distance learning courses favor *Second Life* because they feel more "connected" with their peers and the instructors due to its realistic environment, compared to communicating in online chat rooms or similar methods (*18*, *59*, *60*). A gathering of students' avatars promotes a feeling of "social presence." Education researchers view this as especially important in distance learning classes (*61*). Instructors can employ the same lecture and discussion techniques in *Second Life* that they would use in a real classroom, involving just one individual or a large group (*62*).

While it is true that the term "attitudes" can encompass many different aspects of how students view the class and learning the subject matter (*63*), research of virtual worlds generally shows that students have a preference for augmenting their regular classes with activities in virtual worlds or for substituting virtual activities for similar real world assignments (*18*, *21*, *36*, *41*, *53*, *64*). Exceptions to this tendency exist and are related to the student population studied (*65*) or technical problems experienced during the study (*17*). The first two benefits of using *Second Life*, increased comfort and favorable attitude, are expected to lead to a third advantage: higher academic performance. This result is reported in the literature although analysis of student grades or other measures of academic achievement are less often studied compared to attitudes (*21*, *36*, *64*).

Most educational uses of *Second Life* can be placed within one of three categories. Students meet to plan collaborative projects or participate in a discussion. Students create virtual objects in order to learn computer programming or to express their creativity. Third, and most relevant to this book, students immerse themselves within a simulation and interact with other avatars in order to learn another subject. Many SL locations are modeled after historically significant locations in the past and present, allowing students to learn through role playing (*66*, *67*).

Although a rich variety of educational experiences are found within *Second Life*, it is surprising that published reports of science laboratory experiments are almost rare. Many places are devoted to science but their offerings are more akin to a museum in which an avatar moves from one display to another, experiencing through observation but not participation. A list of science-related SL locations can be found online (*68*). A review of the literature found few descriptions of interactive SL laboratory experiences in science courses.

One example of a laboratory activity involved a mix of 110 Masters and undergraduate biotechnology students performing a polymerase chain reaction (PCR) experiment conducted at the University of London (*36*). One group of students viewed a real world demonstration of a PCR procedure while the other group created avatars to perform a virtual PCR procedure within *Second Life*. All students then completed a PCR experiment in the real-world laboratory. Both groups showed similar increases in knowledge based on scores of pre- and post-experiment quizzes but students performing the virtual world-based activity found the real-world experiment easier to perform and strongly felt that the SL activity improved their understanding of the PCR method. Though there were some shortcomings to the study's methodology (e.g. students who arrived on time to class were preferentially placed in the SL experimental group), results of the study suggest that STEM educators can design successful interactive laboratory activities in *Second Life*.

Another potential use of *Second Life* is for safety training for chemistry lab students (*69*). In one activity, students in an introductory chemistry class can enter a virtual chemistry laboratory resembling their actual lab classroom with chemicals and safety equipment found in the same locations. Students' avatars view tutorials about working with Bunsen burners, waste disposal, cleaning glassware and other safety issues. Students complete a multiple choice quiz after viewing each tutorial. This activity was found to be more instructive than viewing a video about the same topics. Training in *Second Life* is not limited to academic labs. Emergency first-responders also train in *Second Life* to help prepare them for natural and man-made disasters (*70*).

A search of funded NSF STEM education projects shows that *Second Life* is the predominant virtual world that educators are studying. All grants which use another immersive virtual environment are studying education in high school or middle school. This makes sense because such research would be difficult to perform in *Second Life* due to its age restrictions. Examples of projects to develop SL laboratory activities include biology field work (*71*), engineering (*72*), and computer science (*73*). Other awards fund projects involving other activities in SL (*74*, *75*). Assuming NSF's current and recently funded projects represent a trend, STEM education in *Second Life* is increasingly common.

The Potential of Virtual Laboratory Experiments in *Second Life*

Although college students do not conduct chemistry lab experiments in *Second Life*, many do perform computer-based virtual experiments. The two most popular commercial products are Late Nite Labs and Virtual ChemLab. Chemical education research for both products show benefits to students. Several articles in the *Journal of Chemical Education* describe students using Virtual ChemLab prior to performing chemistry experiments (*76*, *77*). Its supplemental

In Pedagogic Roles of Animations and Simulations in Chemistry Courses; Suits, J., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2013.

use increased students' academic performance in the lecture class and students gained deeper knowledge of the subject matter, especially for those students who spent the most time using the simulations. Similar findings were noted for another, less sophisticated set of virtual chemistry experiments (*78*). Late Nite Labs advertises itself as an effective replacement for conventional experiments and some research supports this claim. A study of high school students' attitudes and academic performance when performing Late Nite Labs experiments and similar real experiments showed that students generally enjoyed the virtual experiments more and achieved similar grades (*79*).

Given the availability of products like Virtual ChemLab and Late Nite Labs, it is reasonable to ask what particular advantages SL chemistry experiments could offer. *Second Life* is not designed just for performing chemistry experiments. It is designed to be an enjoyable, interactive and immersive experience. The fact that it is a virtual *world* yields many benefits, from students' enjoyment to the long-term sustainability of SL chemistry experiments.

Individuals perform other virtual lab experiments by working separately at their own computers. In SL, avatars can meet in the same virtual space. This not only allows for collaboration (i.e., lab partners working together) but also creates the sense of social presence (*61*). Students typically perform a real world experiment with a partner and alongside their classmates. In this way, an SL laboratory experience is more realistic than a virtual lab software program.

Students will quickly learn that there's a lot more to SL than just virtual experiments. Being in *Second Life* is inherently a social experience with appealing scenery and interesting experiences. Participants might spend extra time customizing their avatar. Students do not have to venture out beyond the SL chemistry laboratory or change the avatar from its default appearance but it is likely that many will spend more time in SL than required (*18*, *19*, *34*). An educational software program does not offer its users this level of immersion.

Development and improvement of stand-alone virtual lab software requires a significant investment which only the program's creators can make. The SL platform and tools already exist for users to create content for free and they are continuously updated by Linden Labs. A community of educators and other users provide their own expertise to improve the SL learning experience. For instance, Kemp, Livingston & Bloomfield (*80*) developed *Sloodle* to integrate *Second Life* with the *Moodle* learning management system. Students in SL can talk with students logged into a *Moodle* chatroom. They can take a quiz in *Second Life* and the grades are posted in the *Moodle* grade book. *Sloodle* makes certain actions in SL easier by providing toolbars added to the SL Viewer and many other features. Once the benefits of SL chemistry experiments become apparent, other educators will direct their creativity towards developing new virtual experiments in the same way that many already provide SL tutorials, listservs and other tools.

Second Life is known to those with just a passing interest in technology. A slight familiarity should spark more interest in students than a new, unknown chemistry computer program. Students may know about *Second Life* because their other professors use it too. The many citations provided in the earlier section demonstrate that SL is an increasingly common platform for learning in many subjects.

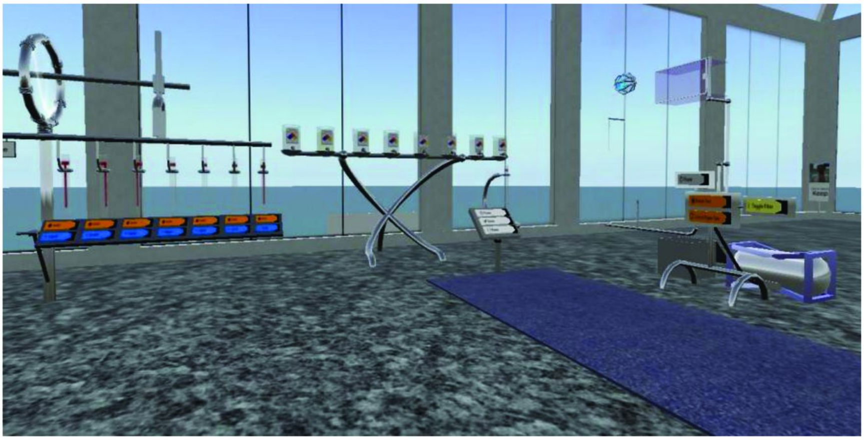

Figure 2. A qualitative analysis experiment with test tubes for mixing solutions (left), a row of reagents (middle) and a flame testing apparatus (right). (see color insert)

Colleges and universities are focusing on distance learning to attract students located far from the school and using of technology to improve access for students on campus as well. It is worth noting that most of the citations for SL education are in non-STEM fields, with some exceptions. One possible reason for STEM educators lagging behind this trend is the need for laboratory activities. Options for conducting a distance laboratory course are limited. STEM educators need to design more ways to offer such courses in order to meet the needs of a growing population of students. This expansion of chemical education opportunities will primarily impact women since they comprise 67% of all distance learners in the United States (*81*). Students with physical disabilities are more comfortable performing activities in virtual worlds (*82*). Well designed SL chemistry experiments can provide more students with access to a high quality laboratory education.

An informal survey of twenty three public and private universities in the US southeastern region shows an average lab fee of $45 per student, per semester for a 1-credit general chemistry lab course (*83*). The cost to students ranged from 0 to $150. *Second Life* chemistry experiments could not only lower the cost to students but also relieve some of the stress on many chemistry departments' lab budgets. Virtual experiments yield no chemical waste and there are no costs associated with laboratory equipment maintenance or breakage. Since students can complete their lab assignments at a computer rather than in a teaching laboratory, virtual experiments can allow schools to schedule more chemistry lab sections in order to relieve overcrowding in the teaching laboratories. Virtual laboratory experiments could therefore improve the quality of teaching in other real world laboratory class as well.

Experiments in an SL chemistry laboratory can involve all manner of instrumentation, dangerous reaction conditions and unusual environments that are not available for real world experiments for obvious reasons. What could

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students learn by analyzing Martian soil for organic compounds, studying the heat of reaction of rocket fuel or detecting air pollutants using a GC/MS? It is not even reasonable to ask such a question for a typical general chemistry laboratory but an LSL programmer can build an experiment that includes anything.

In order to demonstrate the potential value of SL chemistry experiments, the author has developed experiments covering the following general chemistry topics: qualitative analysis of cations, measurement of heat of combustion and determination of a rate law. The experiments not only mimic the real experiment procedure but also generate realistic data and duplicate other features of a student's typical laboratory experience. A video demonstration of the kinetics experiment is available online (*84*). The workspace for qualitative analysis in *Second Life* is shown in Figure 2.

The virtual experiment begins when a student's avatar approaches the lab bench and selects the option to start the experiment from a control panel. Before working with any of the equipment and chemicals, the student must complete a pre-lab quiz conducted in SL consisting of five multiple choice questions randomly selected from a question pool. Once complete, the avatar performs tasks when the student clicks on an item with the mouse pointer. This causes a menu of options to appear in the SL Viewer screen. Options for a graduated cylinder might include "fill with 0.1 M HCl" or "pour into beaker". Once the student selects a menu option, the item then moves and performs the selected action. Avatars can control instrument settings by pressing buttons and turning dials. Information such as time or temperature appears on a small monitor screen next to the instrument. A student can click on a control panel button that opens a MS Word file (loaded outside the SL Viewer) containing the experiment handout or a spreadsheet for recording and graphing data.

There are many ways that a real experiment can go wrong due to incorrectly assembling the apparatus or skipping a step in the procedure. All such errors are possible in the SL experiments also. Students can still proceed after they unknowingly make a mistake and they will generate data that reflects their error. In fact, even when they perform the experiment correctly, their SL experiment data will show some random error. Students record their own data and analyze it after completing the experiment, just as they would for any real lab exercise.

A script at the experiment station records the avatar's name and each action performed during the experiment. This allows students to complete their lab work unsupervised if desired. Instructors can receive an email indicating that a user attempted the experiment and read a list of the actions taken by each avatar. This verifies that the student actually performed the entire procedure and can help the instructor see where a student made a mistake. For some experiments, such as qualitative analysis, one goal is to identify unknown species. At the beginning of that experiment, a script randomly selected cations that appear in the student's unknown solution. Afterwards, the student's avatar selects the ions believed to be present. A script immediately evaluates the student's selection, provides feedback via a message displayed on the SL Viewer and sends the results to the instructor.

In the summer of 2011, Mr. Matthew Scott and his high school chemistry class met the author in a chemistry laboratory located on ACS Island within *Second Life*. This "field trip" was part of their laboratory work at the School of Science and Technology in San Antonio, Texas. Mr. Scott's students would be the first to perform realistic chemistry experiments in this virtual world (*85*).

Five students performed the Rate of Reaction experiment. This experiment allows students to determine the order of reaction with respect to magnesium metal and hydrochloric acid, the rate constant value, the activation energy and the pre-exponential factor contained within the Arrhenius equation. Students monitored the reaction by measuring the volume of hydrogen gas as a function of time. The gas accumulated within an inverted beaker immersed in a water bath. Students vary the length of magnesium ribbon, concentration of HCl and the water bath temperature. Figure 3 shows a screenshot of a student's avatar performing this experiment in *Second Life*. Both high school and general chemistry students are known to perform this experiment (*86*, *87*).

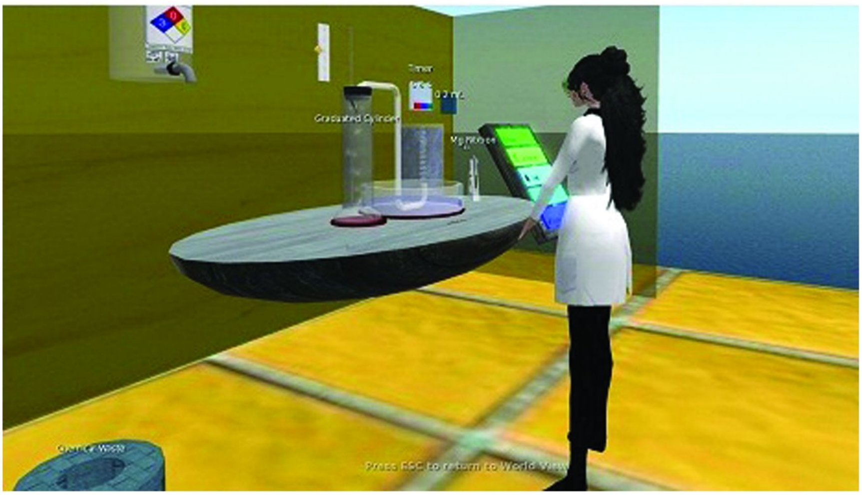

Figure 3. A high school student's avatar performs the Rate of Reaction experiment in Second Life. (see color insert)

A few students initially experienced technical problems accessing *Second Life* due to their school's firewall. Once that issue was resolved, they did not encounter any technical difficulties. Mr. Scott helped them create avatars and taught them to move and function within *Second Life* during the previous day's class session. Students performed the SL experiment, wrote a report and completed surveys to measure their attitudes about completing school work in a virtual world. All students successfully completed the experiment and correctly determined the reaction's rate law and activation energy. Students worked individually, rather than in pairs, but each finished the experiment in less than half the time it took pairs of college students in a real world lab. The brevity of the experiment is due to using keyboard and mouse clicks to perform actions in the virtual world as opposed to handling with glassware and chemicals in a real laboratory. Overall, students enjoyed the lab activity though they favored working with chemicals rather than computers. They found the experiment as challenging as any other real world experiment and were pleased to finish it sooner than expected. A more thorough analysis of this activity will appear in a forthcoming journal article.

The question of whether virtual experiments can replace real chemistry experiments is complicated and remains largely unexplored. First, educators should consider which aspects they value in a laboratory experience – improving students' attitudes about chemistry, reinforcing knowledge of lecture topics, gaining kinesthetic skills, preparing students to perform research or other goals – then determine what types of experiments lead to the desired results. Educators should realistically assess the current state of laboratory education. A curriculum of well-designed inquiry experiments taught by laboratory instructors trained in the appropriate pedagogy may be the best arrangement but it is definitely not the norm. Any comparisons between virtual and real experiments should take this into account. This pilot study is a step towards finding an answer. The author and Dr. Wendy Keeney-Kennicutt are currently investigating the educational value of virtual general chemistry laboratory experiments in more detail.

Conclusions

Virtual worlds provide a new venue for learning, even learning chemistry. Educators are beginning to explore the possibilities for distance learning, role playing and simulations. *Second Life* provides robust features that make it a superior choice among virtual worlds for higher education. The successful performance by high school students in this pilot test suggests that experiments performed in *Second Life* are technically feasible and potentially a useful way to conduct a laboratory class for both students and faculty.

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Chapter 8

Using Virtual Worlds in the General Chemistry Classroom

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The 3D environments of virtual worlds like Second Life (SL) have much to offer a general chemistry classroom instructor, especially when teaching chemistry concepts like VSEPR theory and the 3D nature of molecules. Students can benefit from a variety of synchronous and asynchronous activities within a virtual world, including office hours, videos, simulations, games, quizzes and interactions with virtual chemical species. An extensive mixed methods study compared test results of students who finished three VSEPR-related activities in SL to the results of a control group who did the same activities on paper. Findings showed subtle but significant differences in increased student ability by the SL group for interpreting routine 2D presentations of 3D chemical structures using solid lines, dashed lines and wedges. Although the experimental group attitudes toward SL were split on whether SL was a good idea for a chemistry course, the potential benefit of SL in chemistry classrooms was demonstrated.

Introduction

The general chemistry university classroom is an appropriate and stimulating place to involve the use of a 3D virtual space, like Second Life (SL), whether the class is large or small, on-line, face-to-face or blended. The use of virtual worlds brings an entirely new dimension to teaching and learning (*1*). Developing

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3D spatial awareness in chemistry students, such as understanding the shapes of chemical molecules and ions, would especially benefit from working in a 3D virtual environment.

The Virtual Classroom

Face-to-face (synchronous) activities can easily occur in the virtual world. Instructors can use their virtual selves, called avatars, to directly interact with up to about 40 student avatars directly in several ways, such as text or voice chatting with students (*2*) and conducting PowerPoint presentations using a virtual slide viewer (*3*). SL supports synchronous communication (*4–6*), where an instructor can hold office hours in-world (in SL) (*7*), the class can meet virtually, students can have field trips to any world attractions or museums (*8*), and a conference can take place online (*9*). At Drexel University, faculty administered organic chemistry quizzes (*10*), students played games related to NMR spectral assignments (*11*) and students networked with faculty in chemistry related fields (*12*). SL combines all kinds of computer-mediated communication (*13*). It is even possible to stream the output of a computer desktop with an interactive pen display, like a Sympodium® output, into Second Life. This allows the instructor to work problems on the computer screen and have students see the solutions in-world with only a short delay.

Virtual worlds also support asynchronous activities when the instructor is absent. Students can engage in learning materials designed by instructors, watch videos and PowerPoint presentations, work on virtual assignments (including notecard writings, virtual presentations, object creation, taking photos of their work, etc.), interact with quizzes, chemistry simulations, chemistry games and assignments in-world, in the same way as doing on-line homework. The difference is that students are more engaged since they can meet in groups, like lab partners, in-world and work on assignments together.

An instructor can intentionally design virtual materials to integrate these media so students can be fully immersed in learning. Through synchronous or asynchronous interactions with technological media, students are engaged in inquiry-based (*14*) and student-centered learning (*15*).

There are many professional organizations and resources in Second Life for educators. The EdTech Community on EdTech Island (*16*) has over 2000 members; their goal is to assist teachers in accessing information, share ideas and techniques, and exchange tips with other teachers. The Virtual Worlds Education Roundtable (*17*) with over 600 members, formerly known as the SL Education Roundtable is a weekly meeting for anyone in Second Life who wanted to meet other educators and share experiences. The Applied Research in Virtual Environments for Learning (*18*) has over 100 members and is a special interest group of the American Educational Research Association (*19*). Lastly the Virtual World Best Practices for Education (*20*) has over 600 members; its purpose is to run an annual completely in-world free conference on virtual worlds, best practices and how they are used in education. Another resource is the Second Life Education Wiki (*21*).

The Virtual Chemistry Classroom

Applications of chemistry and chemical education in the virtual worlds like Second Life have been extensively reviewed (*22*). The authors included the visualization of molecules using a rendering program like Orac, a tool that creates molecules using any SMILES, InChi or InChiKey format. Once created, the molecules can be moved, sized and rotated. Figure 1 shows Orac building an acetic acid molecule in real time.

Figure 1. Orac building a molecule of acetic acid.

It is also possible to render chemical reactions in 3D to show conformational changes. The individual work and the collaboration between these two authors provided tools and expertise to encourage faculty to participate and develop virtual world chemistry activities.

Dr. K's Chemistry Place (Figure 2) is on one corner of 12th Man Island, one of several Texas A&M University Second Life regions, called islands. It is divided into two areas – one for general instruction and the other for illustrating and studying 3D molecules and ions with Valence Shell Electron Pair Repulsion (VSEPR) Theory. Its development is described in a blog (*23*).

Figure 2. Dr. K's Chemistry Place (see color insert)

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In the general instruction area (Figure 3) there is a classroom corner which includes a working blackboard, a notice board, a movie screen to show videos and stream a Sympodium® desktop to work on problems in real time during office hours, an in-world clicker system, seating that allows students to raise their hands, and a quizzing system used to generate discussion during office hours.

Figure 3. General instruction area.

During office hours, a headset microphone allows a two way conversation with the instructor speaking without echoes, while students use a chat box to communicate. Most faculty use this combination of communication techniques. One of the most important parts of running office hours or a review session for a chemistry class is being able to work out problems. Wirecast, from Telestream, converts a PC computer into a streaming server. Problems can be displayed on a Sympodium® which then appear on the movie screen in SL with only a few seconds delay. The students must have Quicktime downloaded onto their computers and they must be inside the university firewall. Some students working from home had to set up a VPN (Virtual Private Network) to do so. The SL clicker system (Figure 4a) and the obelisque quizzing system (Figure 4b) work well together to promote student interaction and learning. The quiz system can be used by students even when the instructor is absent. There is more detailed information about these teaching tools on-line (*23*).

Included in the area are chemistry simulations that students can use to better understand certain phenomena. Figures 5a-c shows three interactive chemistry simulations: (a) an interactive simulation linking quantum numbers with orbital shapes, (b) an interactive periodic table, and (c) H_2 absorption spectrum device. There is also room for entertaining, interactive chemistry fun in the area involving moles. Figure 6 shows two games: “How many moles can you find?” and Whack-A-Mole.

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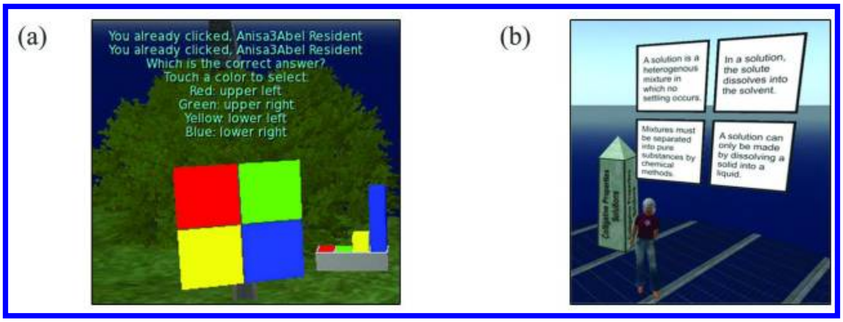

Figure 4. Teaching aids. (a) Clicker system (b) Obelisque quizzing system

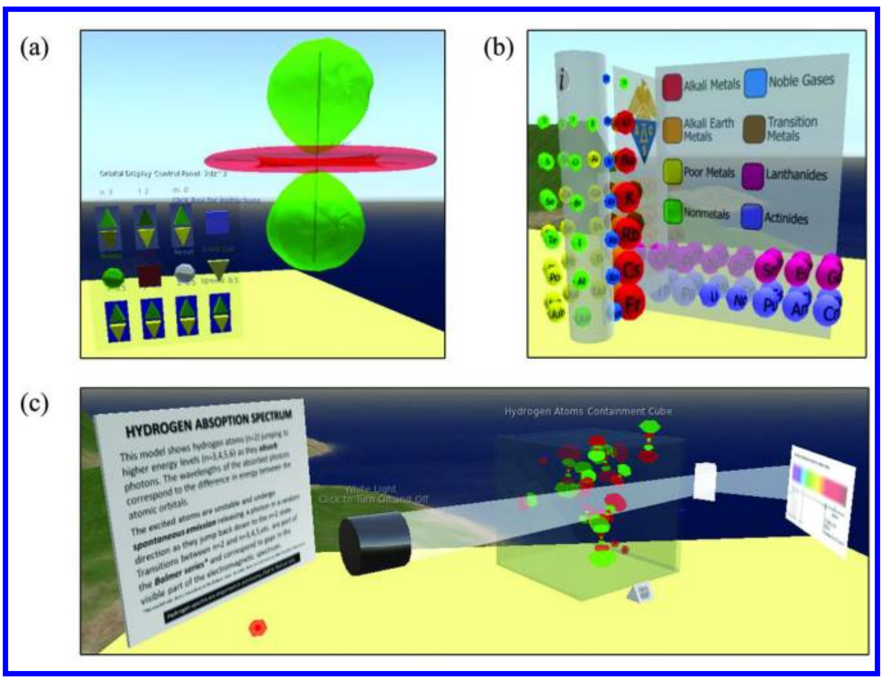

Figure 5. Interactive chemistry simulations. (a) quantum numbers and orbital shapes (b) periodic table (c) hydrogen absorption spectrum device.

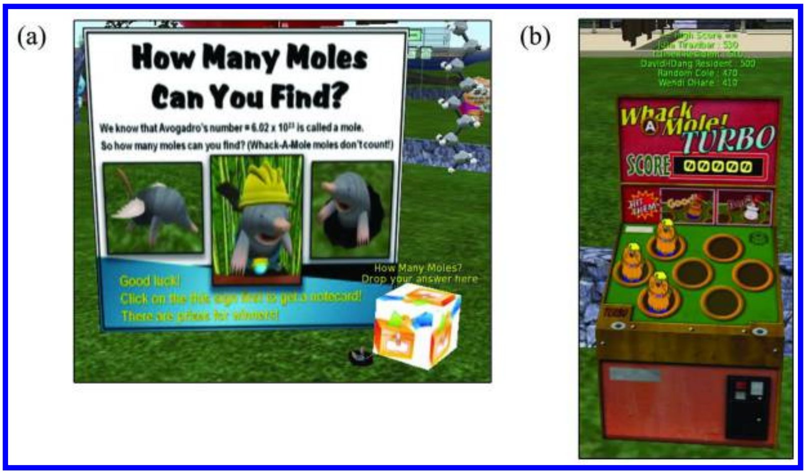

Figure 6. Interactive games. (a) How many moles can you find? (b) Whack-A-Mole

Spatial Ability and Chemistry Understanding

Recent reviews (*24–26*) cite the lack of spatial ability and visualization skills as challenges that students face while studying chemistry. Literature suggests that spatial training and use of molecular visualization in the classroom can lead to gains in student academic achievement (*27–32*). A chemist must be able to visualize the arrangement of atoms in a 3D space to know the shape of molecules. A goal of chemistry instructors is to enhance students' visual and spatial abilities to translate and transform molecules mentally and physically between the 2D and 3D worlds. Students' difficulty in learning chemistry concepts can influence their self-efficacy and their belief that he or she can be successful in accomplishing a task (*33*, *34*). Research suggests that self- efficacy acts as a catalyst in expediting the learning process (*35*, *36*). Therefore, embedding spatial training in chemistry instruction using desktop 3D virtual reality environments' features can play a mediating role in enhancing students' chemistry achievement.

Virtual environments like Second Life (SL) offer a platform for relatively simple development of complex 3D interactive objects, like molecules, without engaging in extensive computer programming. These environments provide an element of "presence," that is reported to improve student learning outcomes (*37*). SL is increasingly used for education, including chemistry, with three benefits: visualization, immersion (presence) and collaboration (*38*). In SL students can combine the macroscopic and particulate worlds of chemistry. These aspects of SL produce at least the same benefit to understanding chemistry as shown by other studies given above. At present, a student can enter SL, create a persona called an avatar, build, and interact with molecules either with SL construction tools from basic SL building blocks, or use newly developed tools which make the creation of 3D molecules easier. Using and understanding effective visualization techniques are critical to a student's success in chemistry at all levels. Tools that assist students in understanding the 3D nature of molecules abound, from

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gum-drops and toothpicks to highly developed and sometimes expensive computer drawing programs and simulations. Second Life (SL) as a platform offers unique advantages over more traditional means that enhance chemistry education: multi-dimensional visualization, immersion, interaction, collaboration, cooperation and team-building.

Virtual reality technologies not only allow students to learn chemistry content, synchronously and asynchronously, but one of the most vital and promising affordances of the virtual reality technologies is to provide spatial instruction. According to Moore (*39*) "….by teaching the students to think in 3D using visualization techniques, their spatial cognition can be enhanced." Similarly, Hedberg and Alexander (*40*) who emphasized the benefit of using 3D virtual reality environments stated, "As ideas are represented in a three dimensional world, three dimensional thinking can be enhanced, and the mental transformation of information from two to three dimensions can be facilitated." Dalgarno, Hedberg, and Harper (*41*) propose that "If 3D environment is a metaphorical representation of abstract ideas, it may be that by developing an integrated database of two dimensional views of a three dimensional model of the concepts, we are better able to make sense of the concepts than through other instructional approaches" (p. 8). So, one of the critical features of 3D virtual reality environments is the ability to visually depict and interact with spatial representations of abstract concepts. Therefore, this feature of 3D virtual environments can be useful in providing instruction for developing spatial ability.

Many studies conducted to examine the effectiveness of virtual reality technologies in chemistry have found positive effects (*31*, *42*, *43*) However, researchers must focus attention on analyzing the role of the mediating variables between the effects of 3D virtual reality technologies based instruction and chemistry learning. These are the variables that attempt to explain how and why the effect occurs. According to Waller, Hunt, and Knapp (*44*), 3D virtual reality technology researchers should explore perceptual and psychological variables that influence learning. Understanding the role of these mediator variables is also important for guiding instructional designers as they create learning modules with the features of virtual reality.

Second Life Chemistry Study

In Spring 2011, a large mixed methods study was conducted at Texas A&M University to investigate the use of Second Life in teaching a particular chemistry topic, Valence Shell Electron Pair Repulsion (VSEPR) Theory, to first semester general chemistry students. VSEPR theory was selected as a measure of chemistry learning because it is one of the most fundamental, abstract, and spatially demanding concepts in undergraduate chemistry courses (*45*), where students are expected to view molecules in a 3D space. It was a quasi-experimental pre-posttest control group research design study using two Chemistry 101 classes with ~240 students in each class. The experimental group did 3 activities in SL over a 6 week period while the control group did the same 3 activities using two 2D rotated screen shot images. The study, including post-tests, was completed

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before the students did a VSEPR laboratory exercise. The data was analyzed for a total of 290 students who completed all three measures. A total of 153 participants were in the experimental group and 137 participants were in the control group. Overall, the participating students were 36% male and 64 % female; 68% were non-chemistry science, engineering and technical majors and 23% were students who had not declared a major. The remaining were students in unrelated majors. The class composition was similar between the experimental and control groups.

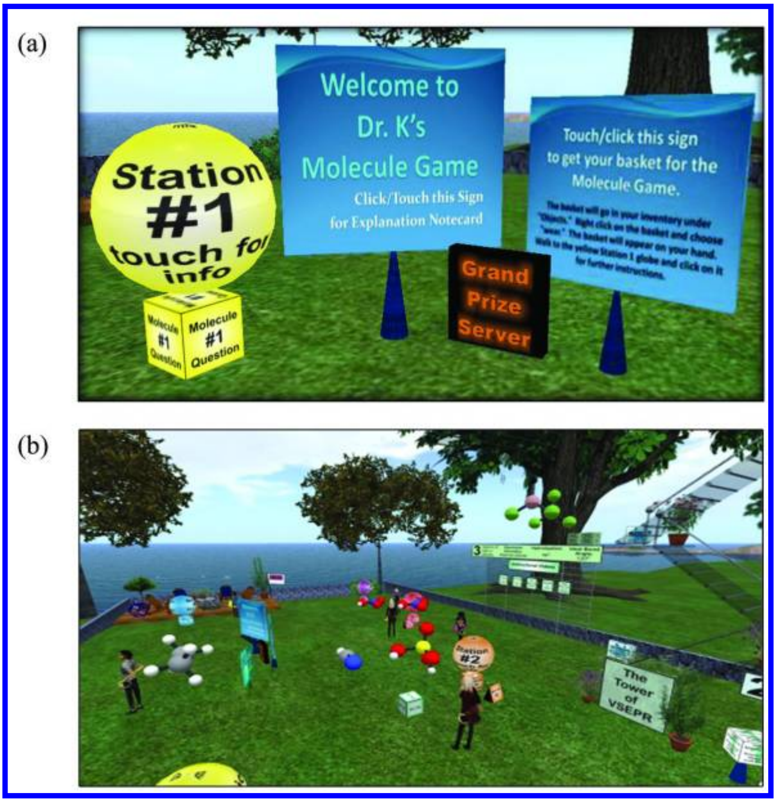

Figure 7. The Molecule Game. (a) The basics of the Molecule Game (b) Students playing the Molecule Game (see color insert)

Activity 1

The first activity, The Molecule Game, was designed for two purposes: (1) to develop SL skills (inventory, chat, interacting with objects, taking photographs) that students would need for the third major activity and (2) to improve students' ability to see molecules in a 3D space from multiple perspectives. Figure 7a shows the basics of the game and Figure 7b shows several students playing the game. Students had to "rezz" (i.e., make an object appear in the Second Life environment) molecules at five different stations and answer a chemistry-related question about each molecule. For example, one of the stations had an ethane molecule. When

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students rezzed the molecule, a note appeared asking "How many hydrogen atoms does an ethane molecule have?" The students could view the ethane molecule, count the atoms, and walk around if necessary to view the molecule from different perspectives in order to answer that question. When the students answered, they received feedback. When finished, the game automatically sent an email to the researchers. In addition, each student emailed a picture of their avatar taken at any one of the five stations with their real name.

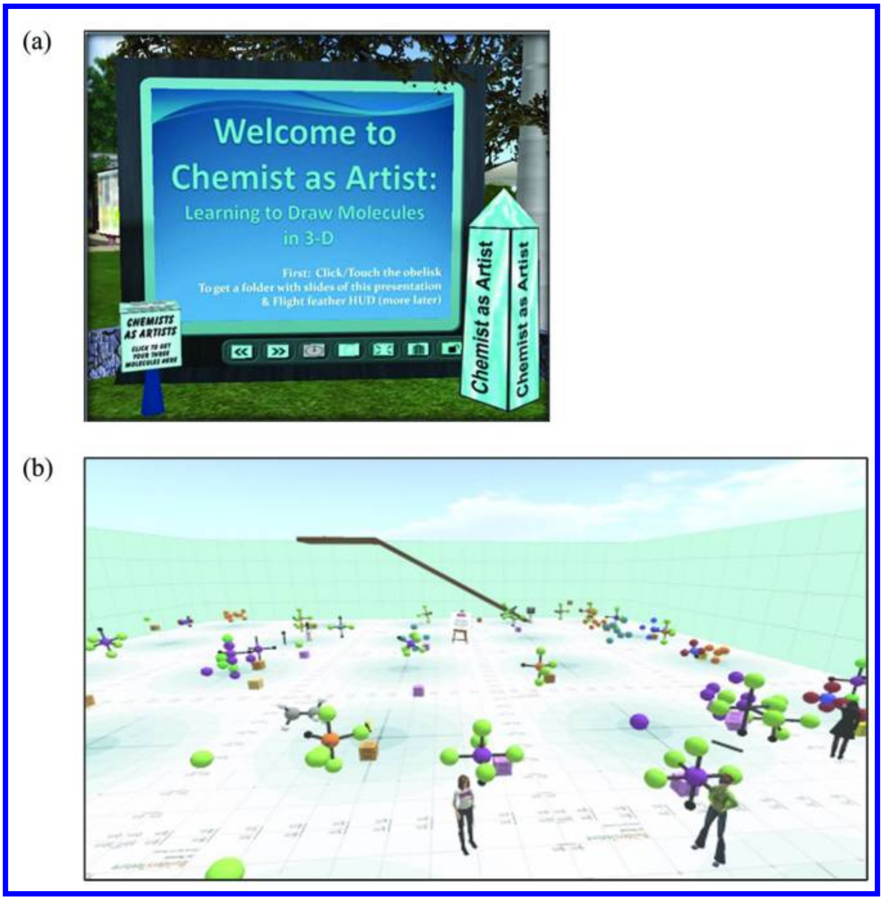

Figure 8. Chemist as an Artist. (a) The explanatory PowerPoint presentation and the molecule giver box. (b) Students rezzing their molecules in the sandbox.

Activity 2

The purpose of the second activity, Chemistry as an Artist (Figure 8a), was to further help students see molecules in 3D by having them draw molecules in perspective using the typical chemistry way with solid lines, dashed lines and wedges. This activity gives the students practice in interpreting 2D representations

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of 3D molecules. Each student in the experimental group was given three VSEPR molecular shapes to manipulate by clicking on a box; the control group students were emailed three pairs of screen shots. For each molecule, the experimental group was required to provide a photograph of their avatars with two orientations and a 2D drawing for each. Figure 8b shows many students in the Texas A&M University sandbox area rezzing their molecules. A sandbox is an area set aside where avatars can build and create. Most islands for educational purposes allow only certain groups to build, but a sandbox allows anyone to build. The sandbox cleans itself every three hours. Dr. K's Chemistry Place allows avatars to build for only 2 minutes, which permits the students to play the Molecule Game. After the allotted time, any build is returned to builder avatar's inventory.

Activity 3

The third activity was an extensive homework assignment on VSEPR theory (Figure 9a). Each student was given 11 different molecules or ions, in either SL for the experimental group by clicking on rotating boxes (Figure 9b) or by email for the control group. The control group was divided into 5 subgroups, with each subgroup getting its own set of 11 species. The experimental group was required to take pictures of two orientations of each molecule whereas the control subgroups were emailed these pictures. Both drew the 2D representations as they did in the previous activity. In addition each student measured bond angles using borrowed protractors, determined electronic and molecular geometries, and drew Lewis dot structures. The molecules and ions were in 6 categories: simple octet obeyers with no lone pairs on the center atom (e.g. HCN, CF_4), complex octet obeyers with at least one lone pair of electrons on the center atom (e.g. NH_3, SF_3^+), simple octet violators with no lone pairs on the center atom (e.g. PF_5, BH_3), species with resonance (e.g. SO_3, NO_3^-), ternary acids and ions (e.g. $HClO_4$, HSO_3^-), and complex octet violators, (e.g. ClF_3, XeF_5^+).

Assessments

There were 3 pre-post timed tests. A 36-question multiple choice chemistry learning test on VSEPR theory was developed, consisting of questions about molecular angles, molecular geometry, and species identification. Three chemistry professors reviewed this test to ensure the validity of the content. The reliability coefficient alpha for the test was 0.90, higher than the acceptable level recommended for learning achievement tests (*46*).

The second pre-post test was the Purdue Visualization of Rotations Test (PVRT). This 20 question test developed by Bodner and Guay (*47*) is a widely used measure of spatial orientation in the field of chemistry. This test has consistently demonstrated a good reliability index ranging from 0.78 – 0.80 in a variety of research contexts. Each question shows a 3D object and participants are asked to select the correct rotated version of the object from the five alternatives provided.

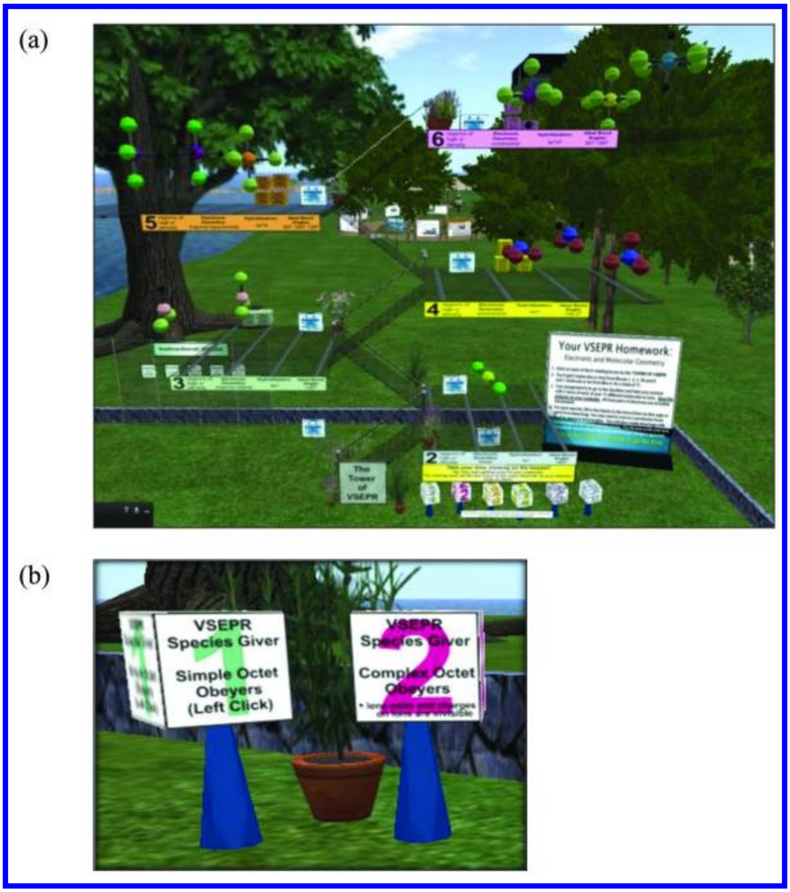

Figure 9. The VSEPR Theory Activity. (a) The Tower of VSEPR (b) Species-giving boxes

The third pre-post test was the Card Rotation Test (CRT) (*48*) measuring mental rotation ability. The students view a random shape and judge which of the eight alternative test figures are either the same, i.e. a planar rotation of the figure, or different, i.e. the mirror image of the figure. It is a 2 page test with each page having 10 reference shapes.

The Test of Logical Thinking (TOLT) (*49*) was given as a pretest to see if both classes scored statistically the same on their formal reasoning ability. Additional posttests included demographics, a presence questionnaire, as well as exam and laboratory grades on the VSEPR topic.

Results and Discussion

Before the interventions, the control group and the experimental group were statistically the same for the VSEPR content test, the PVRT and the TOLT (Table I). However, the two groups were statistically different on CRT pre-test with 160 items (Table II), so with this measurement, score gains rather than absolute scores were tracked.

Table I. Pretest Results

TEST	*Control (N=137) Mean (SD)*	*Experimental (N=153) Mean (SD)*
VSEPR Content Test (36 items)	7.08 (3.56)	7.39 (3.77)
PVRT (20 items)	12.36 (3.48)	11.86 (3.70)
TOLT (10 items)	6.43 (2.10)	6.14 (2.24)

Table II. Results for Card Rotation Test (CRT) Pretest, Posttest and Gain

CRT (160 items)	*Control Mean (SD)*	*Experimental Mean (SD)*	*p*
Pretest	107.9 (30.4)	100.3 (27.9)	0.027 (2-tailed)
Posttest	127.2 (29.5)	123.8 (22.5)	0.28 (2 tailed)
Gain (over 6 wks)	19.3 (20.4) $p<0.001$ Cohen's d=0.64	23.5 (17.8) $p<0.001$ Cohen's d=0.93	0.029 (1-tailed) Cohen's d=0.22

The overall results were subtle, but important. No statistical differences were seen between the experimental and control groups on PVRT and content-based assessments (study activity scores, VSEPR reports done in lab, VSEPR-related exam questions, and the VSEPR content test). This was expected as care was taken to ensure that both groups were given the same instruction on VSEPR-related material. Graduate students were enlisted to time each part of the VSEPR-related instruction in both classes and found no bias. However, the experimental group did show greater statistical improvement on the Card Rotation Test (Table II).

As stated above, for the VSEPR content test as a whole, the posttest scores were not significantly different (Control: 18.41±7.60; Experimental: 18.67±8.73), but in student ability to visualize 3D molecules and bond angles as measured by Part 1 of the VSEPR content test, there was a significant difference (Table III). This skill is a critical component for success in upper level chemistry classes. Part 1 of the test asked students to interpret a 2D representation of a 3D molecule by identifying bond angles in a figure drawn with solid lines, dashed lines and wedges.

Table III. Results for the VSEPR Test Part 1 Pretest, Posttest and Gain

VSEPR Pt 1 (4 items)	*Control Mean (SD)*	*Experimental Mean (SD)*	*p*
Pretest	1.01 (0.57)	1.07 (0.47)	0.26 (2-tailed)
Posttest	1.74 (1.20)	2.01 (1.19)	0.03 (1-tailed) Cohen's d=0.24
Gain (over 6 wks)	0.74 (1.20) p=0.004 Cohen's d=0.78	0.94 (1.14) p<0.001 Cohen's d=1.04	0.075 (1-tailed) Cohen's d=0.18

These results showed that although the effect is small, the experimental group could statistically better recognize the correct bond angles from typical 2D chemical representations of molecules and that many students in both groups were still treating the representation as 2D, not 3D, after weeks of instruction. The wording of the questions was as follows:

> A typical 3-dimensional representation of a molecule in 2-dimensional space uses wedges for bonds coming toward the viewer, dotted lines for bonds going away from the viewer and solid lines for bonds in the plane of the paper. What is the bond angle (rounded to the nearest whole number) expressed by the red dotted line in this molecule?

The angle choices were 30°, 45°, 60°, 90°, 109°, 120°, 150° and 180°. We also asked about the students' confidence in their answer, which ranged from 0 (not confident at all) to 10 (extremely confident).

Figure 10 and Table IV show the results of the four questions for Part 1 using all of the students in the study that completed this particular pre-post test. In (a) Question 1, students did well at choosing 90° as the bond angle before and after the interventions and were fairly confident in this choice. In (b) Question 2, a bond angle in the trigonal bipyramidal structure was chosen. It illustrated the problem that students have in interpreting these diagrams; students tend not to see these figures as representing a 3D structure drawn in perspective, even after being taught and given practice. Initially 50% of all students chose 45°, interpreting the drawing as being a flat 2D structure. However after the interventions, 30% of students were still making that mistake. These students had difficulty in "seeing" the correct bond angle when an understanding of perspective was required. Question 3 in (c) and Question 4 in (d) also demonstrated the same issue. By the end of the study, both the control and the experimental groups improved; however, the students that participated in SL activities showed a small but significant greater gain in this ability (Table IV).

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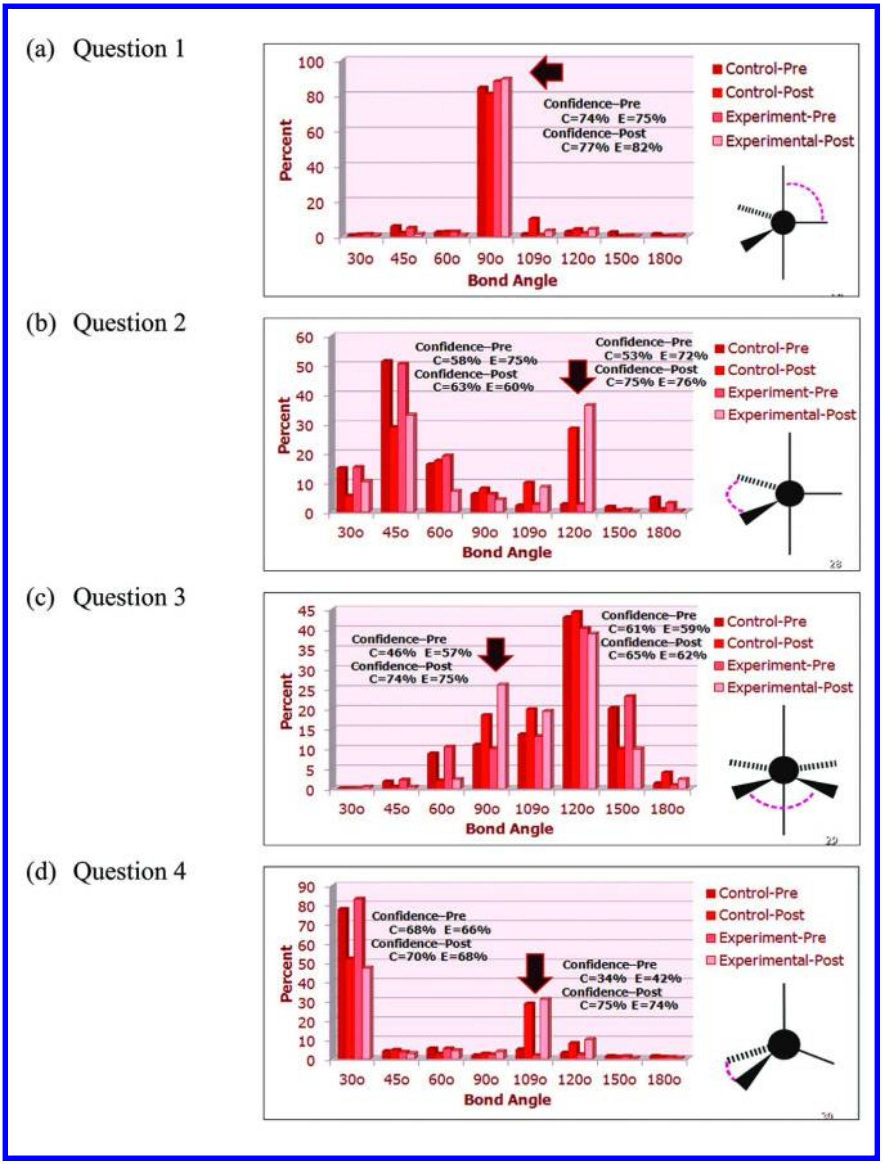

Figure 10. Detailed results for VSEPR pre-post Test Part 1. These are graphs of the percent of students who picked a particular bond angle for the shown molecular shape representation. The average student confidence level is included. The arrow points to the correct answer. (a) trigonal bipyramidal (b) trigonal bipyramidal (c) octahedral (d) tetrahedral.

Table IV. Detailed Results for the VSEPR Pre-Post Test Part 1.

VSEPR Test[a]	*Control (N=194) Mean (SD)*	*Experimental (N=209) Mean (SD)*	*p (1-tailed)*
(a) Question 1			
PreScore	0.84 (0.37)	0.89 (0.32)	0.095
PostScore	0.80 (0.40)	0.89 (0.31)	0.006
Gain	−0.04 (0.49)	+0.00 (0.44)	0.16
(b) Question 2			
PreScore	0.03 (0.17)	0.03 (0.17)	0.45
PostScore	0.28 (0.45)	0.36 (0.48)	0.043
Gain	+0.25 (0.47)	+0.33 (0.49)	0.043
(c) Question 3			
PreScore	0.10 (0.30)	0.11 (0.31)	0.41
PostScore	0.18 (0.39)	0.26 (0.44)	0.034
Gain	+0.08 (0.44)	+0.15 (0.49)	0.064
(d) Question 4			
PreScore	0.06 (0.23)	0.02 (0.14)	0.023
PostScore	0.28 (0.45)	0.31 (0.46)	0.27
Gain	+0.23 (0.44)	+0.29 (0.47)	0.086

[a] Each question was worth 1 point

There was an expected result with the self-reported confidence levels of the students; students who knew the correct answer were generally confident in that answer. Table V gives the mean confidence levels of the more difficult Questions 2-4 for those who chose the correct bond angle and those who chose the most commonly picked wrong bond angle. We saw that confidence levels were not significantly different between the control and the experimental groups. The students who chose the correct answer on the pretest were not sure of themselves with a ~48% confidence level. That confidence level increased to 76% for the students who chose the correct answer after learning about VSEPR theory. The students who picked the most common wrong answer because they apparently saw a simple flat 2D image had no statistical change in their confidence level before and after learning about VSEPR theory, remaining about 65%. These students were fairly confident in their wrong answers, even after extended instruction.

Table V. Average Confidence Percentage on Questions 2-4 for Students Choosing Correct Answer and Students Choosing Most Common Wrong Answer

	Confidence Percent Pretest Mean (SD, N)	*Confidence Percent Posttest Mean (SD, N)*	*p (2-tailed)*
Correct Answer			
Control	47.1 (30.4, N=35)	75.8 (25.3, N=141)	<0.001
Experimental	48.9 (22.7, N=45)	75.4 (23.1, N=193)	<0.001
Most Common Wrong Answer			
Control	64.4 (26.8, N=333)	67.4 (22.1, N=239)	no significant difference
Experimental	64.5 (25.3, N=350)	64.2 (27.2, N=240)	

Further Discussion of VSEPR Pre-Post Test Part 1

The post treatment scores for Part 1 of the VSEPR content test given in Table IV between the control group and the experimental group show small but significant differences, with the experimental group doing better. It is critical to note that even with classroom instruction, access to a 5 minute explanatory video and extensive practice in drawing the structures, the scores for this on-line assessment were low. The students with access to the 3D environment of Second Life did significantly better, but their average post scores were still less than 40% for Question 2-4. Many students were choosing the angle depicted if the drawing were a simple 2D figure. Even with instruction and practice, many students are poor at understanding that the drawing is in perspective.

A retesting of Chem 101 students in Spring 2012 was conducted to see what the results would be after students had completed a laboratory module on VSEPR theory and were tested on their final exam, rather than an on-line assessment. The same questions were used as on Part 1 on the VSEPR Theory test. No required Second Life exercises were assigned. In the lab, students physically built molecules from kits and drew Lewis dot structures, but did not draw 3D representations using solid and dotted lines and wedges. The results were better (Table VI), but still disappointing. There was a weak positive correlation (r=0.50) between final class score and the total score on Part 1 of the VSEPR test. However, when the top half of the class as judged by their final class score was compared to the bottom half of the class, large significant differences were found.

Table VI. Results of VSEPR Test Part 1 for a Different Class (Spring 2012) according to Class Standing.

	Q 1[a] mean (SD)	*Q 2[a] mean (SD)*	*Q 3[a] mean (SD)*	*Q 4[a] mean (SD)*	*Total Score mean (SD)*
For class (N=433)	0.95 (0.22)	0.51 (0.50)	0.42 (0.49)	0.52 (0.50)	2.41 (1.30)
For top half of class	0.96 (0.20)	0.70 (0.46)	0.61 (0.49)	0.74 (0.44)	3.01 (1.17)
For bottom half of class	0.94 (0.24)	0.33 (0.47)	0.24 (0.43)	0.31 (0.45)	1.83 (1.15)
p (2 tailed)	0.43	<0.001	<0.001	<0.001	<0.001
Cohen's d (effect size)	not significant	0.80 (large)	0.80 (large)	0.97 (large)	1.02 (large)

[a] Each question was worth 1 point

It might be deduced that (1) the ability to visualize molecules in 3D is innate, allowing certain students with this ability to do better in this area of chemistry and/or that (2) it might be possible to teach students how to interpret these drawings, since better students academically do better at understanding these drawings. Either way, chemical educators should consider incorporating exercises which allow students to practice interpreting these drawings which are so common in chemistry literature and which professional chemists interpret without difficulty. If many general chemistry students still view these line-drawings as simple 2D figures, instead of representing 3D molecules even after instruction, then they will probably continue to struggle with visualizing these structures. This would affect their ability to succeed in other chemistry-related courses and careers, including biology, organic chemistry, biochemistry and medicine. This study indicated that when students spend time in the 3D virtual world, interacting with objects like molecules, they continuously translate the 2D images they see on the computer screen into a 3D virtual world. Students unconsciously use perspective, the relative size of objects and how molecular angles change in 2D to navigate the virtual space, thereby learning how to convert 2D images into 3D mental models. Even with a relatively short period of time in Second Life as in this study, the experimental group showed more improvement than the control group in their ability to deduce bond angles from 2D perspective drawings.

Future studies could attempt to decipher if the overall poor performance in recognizing bond angles in these drawings is related to such variables as having misconceptions about interpreting the diagrams, poor study strategies, or lower spatial intelligence.

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Student Views of Second Life

To better understand the student perspective on Second Life, two questions posed to the experimental group were analyzed, one quantitative and one qualitative: (1) Is it a good idea to use Second Life in future chemistry classes, and (2) please explain your answer. Question (1) was on a 5 point Likert scale. The results in Figure 11 show that the students were split in their opinion of SL with 41% saying they either agreed or strongly agreed that SL should be used and 37% stating that they disagreed or strong disagreed with the statement.

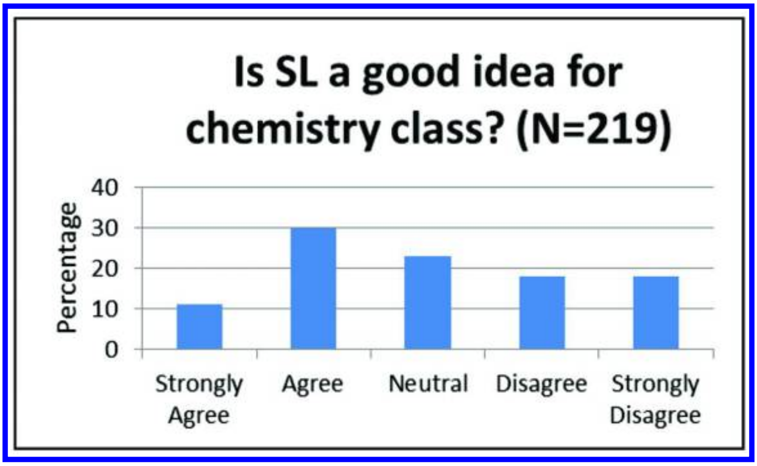

Figure 11. Student Survey Results for Quantitative Question (1).

When students were asked to explain their answer to Question 1, we received 203 replies, with 100 responses dealing with the main theme of perceived usefulness: 58 positive, 35 negative and 7 unsure. Positive points included the ability to visualize molecules (38%) and interactivity (17%). Student statements that speak to the positive aspects of SL usage are:

- It helped a lot with the VSEPR theory by allowing me to visualize the molecules so when I'm drawing them on paper I can see the molecule in my mind's eye. This allowed me to draw 3D molecules faster and easier.
- Being able to modify and view a 3Dimensional representation of a molecule is very helpful when trying to learn to identify those models.
- You can clearly rotate angles and see molecules in a different perspective. That helps.
- It allows you to actually see and interact with a molecule.
- Having seen the molecules in 3D on Second Life, it is much easier now to picture them in mind when they are presented to me as 2D drawings or just given the name of the shape. Besides making my computer run a bit slower, Second Life helped me see the molecules much easier in my mind.

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The subthemes for the students who viewed the SL experience negatively included time consumption (29%) and the fact that other methods of teaching VSEPR theory, including textbooks, 2D images were just as useful (16%). Here are samples of negative student responses:

- I find it frustrating that I had to learn chemistry in a tedious virtual world rather than doing these assignments much more easily and effectively in the real world.
- It was very frustrating and I dreaded going in to Second Life because everything was very difficult and making sure you had all of the necessary objects was frustrating. I did not like Second Life.
- I felt like second life was just a hassle to get the molecules. I would have learned about it just as easily if I had been handed the molecules on a piece of paper.
- The technology took way too much of my time to figure out. Then to learn the material on top of that was far too complicated and stressful. It was very inconvenient.
- I feel it would be easier to lecture about this material and show students more examples.

In retrospect, there were several reasons that caused the obvious frustration that some students expressed in their comments. Others (*50–52*) have also reported student issues. Introducing new technology into the classroom has always been fraught with peril due to student resistance (*53*), but it was shown that students are willing to take a more active and responsible role in their learning with new technology when they perceive the value of such engagement and are supported in their efforts. In this study, there was a definite learning curve to maneuvering in a 3D world which caused many students to struggle. Learning to navigate in a virtual world takes practice. To counteract this known problem, several Camtasia videos, PowerPoints and handouts were developed to guide students. In addition, regular office hours were held, both in a computer lab and inworld in the Second Life study area. Other students had technical issues either with their computer or their internet connection. Still others procrastinated in completing their assignments and so when more than 30 avatars tried to do the assignment simultaneously, there were complaints of time lags and computer crashes. Assigned times were not given for students to work in the SL area which would have prevented overcrowding. This would be a consideration for future assignments. On the activity design side, although attempts were made to simplify both the way students were given their individual molecules and the molecule building process within Second Life, the process required more skill than many students had or were willing to learn. To solve some of these issues, one year after the study was completed, a free, fully copyable SL molecule building kit was especially created for general chemistry students to easily build a full range of VSEPR shapes for molecules and ions. Figure 12 shows the T-shaped molecule, bromine trifluoride, built with the SL Molecule Rezzing Kit. The hope is that with this kit, students will have fewer complaints and the learning will be at least as effective. Approximately 30 students piloted its use in Spring 2012. Student comments were positive:

- I enjoyed being able to build them ourselves just like you did in class.
- The molecule building kit was very easy to use especially because I watched the instructional video you made online.
- Along with the owls and practice drawings from the homework, the molecule building kit helped me see the structures of the molecules in a more 3D and realistic view rather than just in the textbook.
- Once I figured out how to take a picture of the molecule I built, it was very easy to learn and play with the molecules. I thought the game was very helpful when it came to getting a feel for what the molecule shapes really looked like, and I definitely used SL when studying for the final exam.

Figure 12. SL Molecule Rezzing Kit with bromine trifluoride.

Of the 12 responses to a short survey, eleven either agreed (7) or strongly agreed (4) that the SL Molecule Rezzing Kit was easy to use. The person who disagreed had this to say, "The building kit itself was straightforward enough, but Second Life was hard to get used to, and internet problems could make things worse." The student's statement had more to do with the SL learning curve than the molecule kit. Nine students agreed (6) or strongly agreed (3) that the SL Molecule Rezzing Kit helped them learn VSEPR shapes; three were neutral.

Additional Results

One aspect of this study has been published (*54*) looking at only the experimental group. Its purpose was to examine the impact of 3D virtual reality features on chemistry learning outcomes in relation to the underlying variables: selected perceptual (spatial orientation and usability) and psychological (self-efficacy and presence) variables. The relationships between the 3D virtual reality features and the VSEPR chemistry learning test as it relates to the selected

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variables were analyzed using the structural equation modeling (SEM) approach. This method is a powerful and highly reliable statistical technique for testing and estimating causal relations using statistical data combined with qualitative causal assumptions. In this study, SEM gives a very comprehensive multivariate analysis of the psychological and perceptual processes involved in learning chemistry in a 3D virtual learning environment We found that how easily students managed the 3D software, i.e. its usability, strongly mediated the relationships between 3D virtual reality features, spatial orientation, self-efficacy, and presence. Spatial orientation and self-efficacy had statistically significant, positive impacts on the chemistry learning test. These results indicate that instruction within the 3D environment is effective for enhancing students' chemistry achievement. This study provided a research model that can help increase the effectiveness of desktop virtual reality environments, like Second Life, for enhancing spatial ability and science achievement. The study is the first to test a model of chemistry learning in 3D environments by employing SEM.

Activity 1 of the study, The Molecule Game, is still being used each semester to introduce general chemistry students to working in virtual worlds. Completion of the game as noted by an automated email from the game gives the student the same number of points as two quiz opportunities. Since only 70% of the quizzes count as a grade, students can choose not to participate. Figure 13 shows a graph of the number of visitors during the school year from Fall 2011 through Spring 2012. A visitor counter in the Second Life area daily emails a visitor list. In Fall 2011, 132 out of 505 enrolled students actually finished the Molecule Game and in Spring 2012, 151 out of 463 enrolled students completed the game. From the tallied numbers, it is assumed that many students stopped by more than once, and non-students visited as well, since the site is open to all.

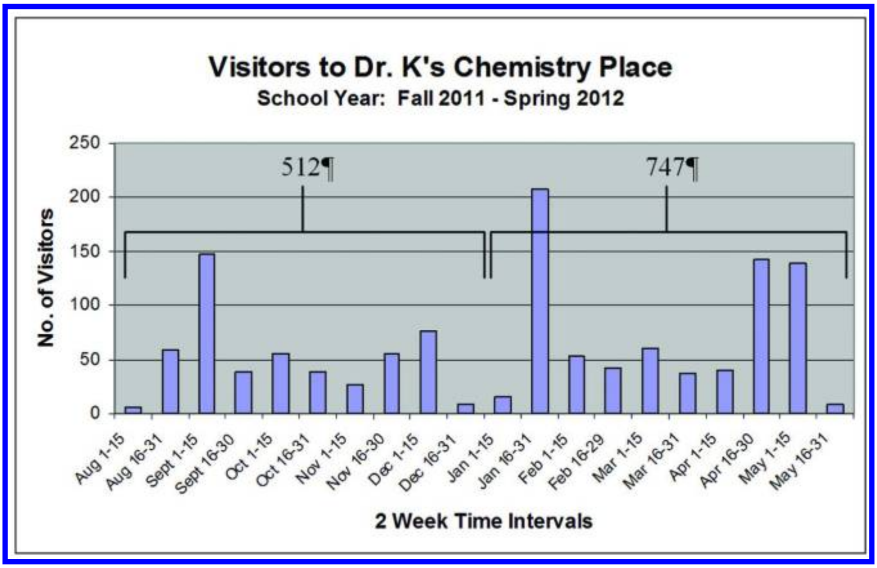

Figure 13. A graph of the number of visitors to Second Life Study Area from 8/1/2011 to 5/31/2012.

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Summary

The 3D environment of virtual worlds like Second Life has much to offer a chemistry classroom instructor, particularly when teaching chemistry concepts like VSEPR theory and the 3D nature of molecules. We have shown that general chemistry students can benefit from a variety of activities within a virtual world, including office hours, simulations, and interactions with chemical species.

Acknowledgments

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Chapter 9

How a Qualitative Study with Chemistry Instructors Informed Atomic Level Animation Design

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As we move forward in an era of electronic instruction and homework, instructors will be relying more and more on visualization tools to help their students independently learn chemistry. As a result, it is very important for instructors to thoughtfully consider the kinds of visualizations they should share with their students to enhance learning. Likewise, it is important for visualization designers to look for direction from instructors when they construct learning tools. This qualitative research study shares insights into the development of atomic level visualizations. The study explores how pictures constructed by nine chemistry instructors were analyzed to inform the design of visualizations. It also focuses on the rationale three general chemistry instructors used to construct their atomic level pictures, and the level of details they expected their best chemistry students to convey. The instructors' contrasting views were used to construct visualizations that scaffold the portrayal of atomic level features from simplistic, where only the most necessary features were portrayed, to complex, where more scientifically accurate features were represented.

Introduction

Visualizations and animations refer to linked representations of phenomena at the molecular, macroscopic and symbolic levels that demonstrate changes in

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scientific phenomena over time (*1*, *2*). Visualizations are sometimes viewed as being more interactive; however, this is not always the case. In this paper, the terms visualization and animation will be used interchangeably.

Visualizations of atomic level events are useful tools for teaching general chemistry students about unobservable chemical phenomena as they provide concrete visual models for open discussion. Many studies report that students who view atomic level visualizations demonstrate better understanding of particulate level phenomena (*3–10*). When instructors teach with visualizations, they likely choose the visualization based on their instructional goals. For example, the visualization may showcase the atomic level events better than the instructor could represent through a drawing or it may show features, such as movement or interactions, that instructors want to emphasize and discuss with students. Regardless of the reason the instructor chooses to use the visualization, a question to consider is: How should designers construct the visualizations?

Visualizations do not come with user manuals that share the designer's motivation for making them. As a result, we do not have insight into the learning theory associated with the design of visualizations or the vision for how the tools were intended to be used. It is likely that many visualizations were constructed to reflect their designer's understanding and the key features he/she wanted to convey. The problem with this approach is evident at any forum where visualizations are shared. Not all professionals agree on what features should be modeled for the student audience. Instructional motivations for using visualizations can vary. For example, some instructors may want visualizations to reflect the latest scientific theories with accuracy, because they do not wish to give students incorrect information or present them with an overly simplified perspective. Other instructors may wish to help students bridge from one level of understanding to another with less regard for the accuracy of all of the events portrayed. For example, in the case of precipitation reactions, the instructor may focus on how some ions attract to form a precipitate, but they may de-emphasize the role of water. It is apparent that a range of complexities can be found in visualizations, and the question becomes how should we determine the amount of information or details conveyed in the tools?

Instructors' Perspectives

In the book "*The Chemistry Classroom: Formulas for Successful Teaching*", Dudley Herron stated, "...we learn a great deal about teaching and learning through our experience with students" ((*11*), p. 17). To build on this quote and connect it to this research, we can learn a great deal about animation design from instructors' experiences with students. A reality of the design process is that instructors need to see the pedagogical benefits of the tools. Teachers' beliefs and personal goals shape their decision on how to use software (*12*). Specifically, their beliefs about how students learn, and their roles as teachers influence their software use. In addition, experts can offer unique insight into the design process due to their mastery of the material and their teaching experience. Studying the instructor's perspective or pedagogical content knowledge provides insight into how he or she makes sense of chemistry concepts to make decisions on what to share with

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beginning chemistry students. After careful analysis of the details desired by experts, a scaffold can be designed that guides students from simplistic conceptual details, where many students begin when they take their first chemistry course, to include more complexities.

Scaffolding

To learn from visualizations, Chiu and Lin state that students need cognitive understanding of the phenomenon as well as metacognitive skills to guide their learning (*1*). In order to assist students in their cognitive development, scaffolding is a tool that can be used to help students actively engage in work and it promotes self-sufficiency. Scaffolding is a support strategy that evolved from examining how human mentors assist students to enhance their range of learning (*13*). Software tools or programs can offer similar mechanisms of assistance to support learning through "structuring the task" and "problematizing aspects of subject matter" (*14*). There are many ways that software tools can give structure to a task or concept. For example, structure can be provided by giving explicit directions, narrowing choices, inviting reflection of understanding, monitoring progress, breaking a complex event into simpler segments or highlighting specific details of an event (*1*, *13*, *14*). In addition to providing structures to bring about better understanding, provoking problem-solving behavior is also desirable, because it tests whether students can proceed independently once the scaffolding is removed. "Problematizing" consists of several characteristics: Introducing a problem or a discrepant event, inviting students to think about aspects of the problem and inviting them to resolve an issue (*14*). Ultimately the aim of scaffolding in the design of animations is to find ways to present the nature of chemistry concepts to shape the students' ways of thinking and learning.

Research Questions

The goal of this study was to examine the key features instructors hoped their best students would convey about the atomic level details associated with substances that are tested for conductivity. Ultimately, these features were used to inform the construction of scaffolds for atomic level animations of conductivity concepts. A phenomenographic approach was used to generate a detailed account of the instructor's rationale for constructing pictures that illustrate what their best students should be able to construct to explain the conductivities of various substances. The specific research questions were:

1. What key features do instructors portray in their drawings when they are asked to illustrate events through the eyes of their best students?
2. What is the rationale behind the types of features the instructors' convey?

The variations in instructors' representations were then used to inform the scaffolding of conductivity concepts into atomic level animations.

Theoretical Framework

The study was qualitative in nature, as instructors used a click and drag tool to construct pictures showcasing atomic level details of various substances that they then discussed during a semi-structured interview. The pictures and interviews were analyzed and coded for key features, and they were also coded to learn the instructors' rationale for their picture constructions.

The theoretical framework that was used to guide this research was based on phenomenography. The aim of phenomenography is to define the different ways in which people experience, interpret, understand, perceive or conceptualize a certain phenomenon in the world around them (*15*). It is concerned with describing aspects of the world as it appears to the individual (*16*). Phenomenography provides the opportunity to contrast different ways of understanding what is ostensibly the same phenomenon in order to highlight features of the phenomenon (*17*). The focus of this study was focused on instructors' perceptions of a specific chemistry phenomenon. The goal was to learn how instructors' conceptualized the features their best general chemistry students should convey in modeling a comprehensive understanding of the atomic level details of a substance's behavior before and after being tested for conductivity.

While this theoretical framework was based on phenomenography it more accurately reflects the knowledge-in-pieces perspective, in which knowledge is constructed on the fly drawing on implicit cognitive elements (*18*, *19*). The aim of the knowledge-in-pieces epistemology was to understand how students learned physics, but Taber and Franco demonstrated that the knowledge-in-pieces framework can be adapted to understand how students learn chemistry (*18*). diSessa developed the framework to understand "the intuitive sense of mechanism that accounts for commonsense predictions, expectations, explanations, and judgments of plausibility concerning mechanically causal situations" (*19*) diSessa states that the knowledge-in–pieces framework reveals "a coarse level of detail" through asking questions to learn:

> *What are the elements of knowledge; how do they arise; what level and kind of systematicity exists; how does the system as a whole evolve; and what can be said about the underlying cognitive mechanism that are responsible for the normal operation of the system and its evolution (19)?*

As previously mentioned the information used to inform the design of the visualizations came from asking instructors to contemplate what pictures made by students with a good understanding of the material would look like. The pictures were analyzed for key features that instructors expected students to know and demonstrate. Instructors drew upon their teaching experiences and their personal learning experiences to construct the pictures and addressed how the elements arose. In this way, the instructors came up with "a *sense of mechanism* – a sense of how things worked" and the elements that were most necessary for students to report to convey this understanding (*19*).

Methodology

Prior to embarking on this study, the researcher reviewed the literature and conducted interviews to gain an understanding of the visualization needs of general chemistry students. However, the researcher felt that in order to best design visualizations of chemistry events, it was also important to examine what it was that instructors expected their students to understand about these chemistry concepts. The goal was to develop visualizations that fit with instructors' pedagogical expectations.

To begin the study, nine instructors were emailed an invitation to participate asking them to complete electronic worksheets that would be used to inform the design of atomic level animations. In the email they were given information on how to access a link to electronic worksheets and they were instructed to complete the worksheets prior to attending an interview session. The electronic worksheets, which were developed by the author and her colleague, involved using click and drag tools to move images of atoms, ions, or molecules from a toolbox to a blank box to construct atomic level pictures (Figure 1) (*20*). A similar tool, designed by Tasker, was created to help students build representations of aqueous ionic solutions (*2*, *21*). Our electronic worksheets differs from Tasker's Molecular Level Construction Tool in several ways. Our electronic worksheets have more atomic level options for the user to click and drag to construct their picture, including unconventional choices presented to capture the user's misconceptions or preconceived notions. The worksheets enable the user to build representations of substances other than aqueous ionic solutions, and they examine how samples respond when a conductivity tester is introduced.

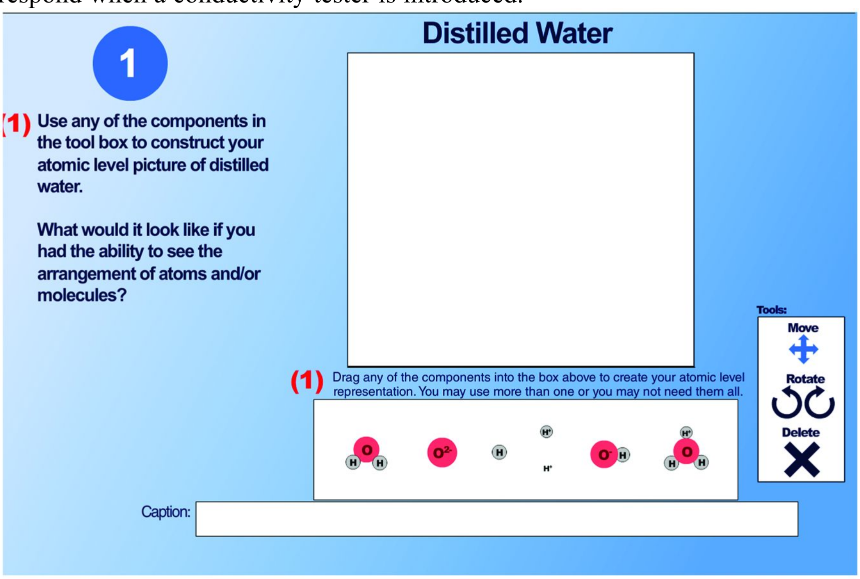

Figure 1. A still image screen shot of the electronic worksheet used to constructing an atomic level picture of distilled water. Reproduced from reference (20). Courtesy of Resa Kelly.

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In the study, instructors were asked to represent the details they would expect their best first semester, general chemistry students to communicate about the atomic level behavior of two chemical substances: Liquid state distilled water and solid sodium chloride. They were also asked to construct the atomic level features of these substances and an additional solution, aqueous sodium chloride, when a conductivity tester was introduced to the substances. Upon completion of the worksheets, instructors were requested to printout their pictures and bring them to an interview session where they would be discussed. As a result, some instructors printed their work in color while others printed in black and white. Semi-structured interviews were conducted to allow instructors to orally explain their pictures, to gain deeper insight into what their expectations for students involved and to learn what key features they chose to emphasize in their representations. The primary assumption of this study was that instructors' conceptions were the product of interactions they had with students learning chemistry. The main result of the research was the identification of features that could be categorized as simple and complex and that could be used in the design of visualizations.

Electronic Worksheet Segments and Scaffolds

Electronic worksheets used in this study were designed to scaffold the conductivity of aqueous sodium chloride into three segments. To recognize that an aqueous solution of sodium chloride conducts electricity, but neither of the substances used to make the salt solution, pure water and solid sodium chloride, conduct electricity before they are mixed, was considered to be a discrepant event for students. Thus, the segments that led up to analyzing why an aqueous salt solution conducts involved demonstrating how each of the mixture constituents behaved before they were mixed and how an aqueous sodium chloride solution responded when tested for conductivity. The third segment addressed how the mixture of salt and water responded when tested for conductivity. The experts were asked to construct these segments based on how they thought the best students would respond to the task. This was done to provide a framework for the instructors and to prevent them from going into depth that was far too advanced for the general chemistry audience. As mentioned, a goal in animation design is to scaffold student learning to provide supports that enable students to better understand the complex content (*14*). Thus, this study will demonstrate how instructors' contrasting views of complexity can be used to inform animation design.

Participants and Setting

The participants consisted of seven male and two female instructors from the same academic institution located in the Western United States. All nine instructors had attained doctorate degrees in a chemistry discipline, six of the instructors had taught general chemistry in the past, but only three instructors had taught general chemistry either one semester prior to or at the time of the study. The nine instructors' constructed pictures of the event segments and their oral explanations were analyzed for key features. From analysis of the nine transcribed

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semi-structured interviews it was observed that three instructors (X, Y and Z) with recent teaching experience were much more in tune to the instructional needs of the general chemistry audience often relating how their constructed pictures reflected their interaction with general chemistry students. As a result, these three professors were purposefully selected as the focus of phase two of the study. Interviews with these professors provided a rich description of the key features they felt students should convey when constructing atomic level pictures of substances tested for conductivity.

Data Analysis

In a phenomenographical analysis, "...we are looking for the most distinctive characteristics that appear in those data; that is we are looking for structurally significant differences that clarify how people define some specific portion of the world" (*16*). In the first phase of the study, nine instructors' constructed pictures and oral descriptions of their pictures were analyzed to reveal their conceptions of how their best general chemistry students should be able to model atomic level details regarding substances before and after being tested for conductivity. The pictures and oral descriptions provided insight into instructors' perceptions of students' learning capabilities. All nine instructors' drawings were scanned into a digital format and analyzed for key features. The key features were created by reviewing and coding the pictures and oral descriptions numerous times, adjusting the descriptions of the key features, and recoding until the system of features stabilized.

In order to study instructors' rationale for making their pictures, audio-recorded interview sessions were conducted. Initially, all of the transcribed interviews were highlighted and notations were made next to relevant statements to organize and prepare the interviews for data analysis. Review of the nine transcripts revealed that oral explanations made by instructors immersed in teaching general chemistry at the time of the study were particularly rich. As a result, the interviews and constructed pictures involving these three instructors were the focus of the second phase of data analysis. In the second phase, themes from the three instructors' pictures and interviews were constructed through a constant comparative method of data analysis where continuous comparison of instructors' constructed pictures and oral responses were made to determine attributes that should be emphasized in the design of visualizations (*22*).

Results and Discussion

Phase 1: Analysis of Chemistry Instructors' Atomic Level Pictures

Nine chemistry instructors (assigned letter identities) were asked to construct atomic level pictures of liquid state distilled water and solid sodium chloride to represent the key features above average general chemistry students should be able to convey after taking a first semester general chemistry course (Table 1). Additionally, they were asked to model the features of distilled water, solid sodium chloride and aqueous sodium chloride after a conductivity tester was introduced into the samples. Their pictures gave insight into the key elements and the mechanisms students should understand about the atomic level nature of these substances (*19*).

Table 1. Essential Features of Samples Tested For Conductivity.

Description of Key Features	*Instructors (9)*[a]									
	A	*B*	*C*	*D*	*E*	*F*	*X*	*Y*	*Z*	*Total*
Distilled Water										
Molecules touch or very close together	1	0	0	1	0	1	0	0	1	4
Molecules with space between them	0	1	1	1	0	0	1	1	0	5
Hydronium ion present	0	1	1	1	1	0	0	0	1	5
Hydroxide ion present	0	1	1	1	1	0	0	0	1	5
Intermolecular forces shown	1	1	0	1	0	1	0	0	0	4
Distilled Water tested for Conductivity										
Ions attract to electrodes	0	1	1	1	[b]	1	0	0	1	5
Conducts weakly	0	1	1	1	[b]	1	0	0	1	5
No ions represented	1	0	0	0	[b]	0	1	1	0	3
NaCl(s)										
Entire box filled with ions	0	0	1	1	0	0	0	0	0	2
Rectangle/Square distinctly represented	1	1	0	0	1	1	1	1	1	7
Space between ions	0	1	1	1	0	0	1	0	0	4
Represent charges on ions	0	1	0	1	1	0	1	1	1	6
Molecule (pairs) represented	0	1	1	0	0	0	0	0	0	2
1:1 Ratio of Na^+ to Cl^-	1	0	1	1	0	1	1	1	1	7
Less than 6 of each ion represented	0	1	0	0	1	0	0	0	0	2
6 or more ions/species	1	0	1	1	0	1	1	1	1	7
Lattice arrangement of ions	1	1	1	1	1	1	1	1	1	9
NaCl(s) tested for conductivity										
No conductivity – pictures do not change	1	1	1	1	1	1	1	1	1	9
NaCl(aq) tested for conductivity										
One of each ion represented	1	0	0	1	1	1	0	0	0	4
2 to 3 of each ion represented	0	1	1	0	0	0	1	1	1	5
Hydration spheres (full or partial)	1	0	1	1	1	1	0	0	1	6
Water molecules mixed with ions	0	1	0	0	0	0	1	1	0	3

Continued on next page.

Table 1. (Continued). Essential Features of Samples Tested For Conductivity.

Description of Key Features	*Instructors (9)*[a]									
	A	*B*	*C*	*D*	*E*	*F*	*X*	*Y*	*Z*	*Total*
Highly conducts	0	1	1	1	0	0	0	1	0	4
1:1 Ratio of ions	1	1	1	1	1	1	1	1	1	9
Solvent water molecules interspersed	0	1	1	1	0	0	1	1	1	6
Solvent water molecules present immediately surrounding ion (hydration spheres)	1	0	0	0	1	1	0	0	0	3
Ions move toward respective electrodes	0	1	1	0	0	1	1	1	1	6

[a] The three experienced general chemistry instructors are labeled X, Y, and Z . [b] Instructor E did not complete the electronic worksheet for the conductivity of distilled water.

Distilled Water Before and After a Conductivity Tester Was Introduced

The most noticeable differences observed in the instructors' constructed pictures of distilled water was whether they demonstrated space between the water molecules, showed intermolecular forces and depicted the auto-ionization of water (Table 1). Slightly more than half (five) of the professors chose to represent distilled water with space between the molecules while four instructors chose to represent the water molecules touching or in very tight proximity. Those who favored close proximity wanted to convey a realistic view of liquid state water, while those who constructed larger space between the molecules felt it was simpler and more likely how students would view it.

Five instructors represented the auto-ionization of water when they included at least one hydronium ion and one hydroxide ion in their population of water molecules. Four of these five instructors predicted that students would recognize that the ions or moving charges would cause water to conduct weakly. Instructor F did not represent the auto-ionization of water in his picture of liquid state water because he indicated that it would be insignificant in the sample representation; however, he did include ions in his pictures where the water was tested for conductivity because he indicated that distilled water would weakly conduct due to the presence of ions and he wanted to provide evidence for why this would occur (Figure 2a & 2b). He seemed to be inserting how he would complete the picture and not necessarily how a general chemistry student would view the concepts. Three instructors predicted that students would not represent auto-ionization because the students do a lab where they learn that pure water does not conduct, thus the students would be inclined to believe that no ions were present. It was noticed that instructor E did not complete a picture to represent how water would conduct indicating that it "doesn't really relate to organic chemistry." As an organic chemist, he sometimes drifted from the assigned task and considered what he wanted students entering an organic chemistry course to be able to convey.

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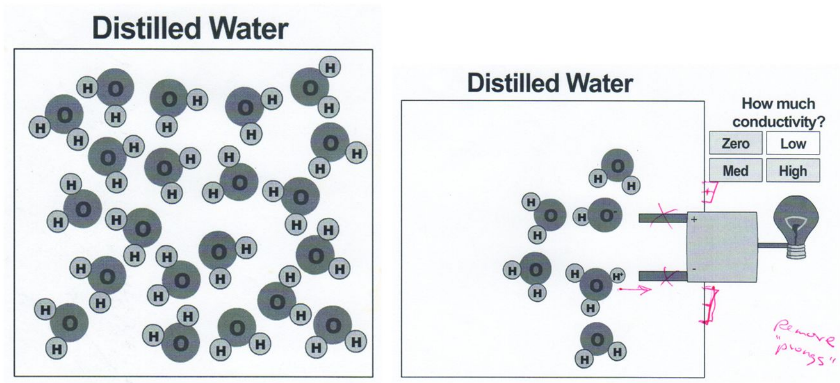

(a) (b)

Figure 2. (a) Example of Instructor F's picture of distilled water. (b) Instructor F's construction of distilled water during a test for conductivity. Note: During the interview Instructor F suggested removing the prongs of the conductivity tester and wrote this on his picture.

Another sophisticated feature that some instructors chose to represent was the presence of hydrogen bonding between water molecules. Hydrogen bonds were evident when instructors systematically oriented all of their water molecules so that the hydrogen ends or regions of partial positive charge of one water molecule were placed near oxygen ends or regions of partial negative charge of another molecule. Those that incorporated hydrogen bonds recognized that this concept was taught toward the end of the first semester, thus they admitted that they would not expect students to recall this feature at the beginning of the first semester.

Solid Sodium Chloride Before and After a Conductivity Tester Was Introduced

In representations of solid sodium chloride, all nine instructors constructed lattice arrangements of the ions in which sodium ions were placed next to chloride ions and vice versa (Table 1). Most (seven) of the instructors chose to represent only enough ions to form a distinct rectangle or square surrounded by empty space to make a connection to the macroscopic cubic crystal state (Figure 3a). Only two instructors completely filled the entire box with alternating ions for a more accurate representation of atomic level solid table salt justifying that a salt crystal was comprised of many ions. Six of the instructors chose ion representations that included charge, but two instructors did not. In addition, there were two instructors (B and C) who represented sodium chloride with molecular pairs. One of these instructors (C) assembled the lattice from molecules of NaCl and indicated that it was more accurate to represent neutral atoms in the lattice due to the nature of interactions between the atoms within the lattice (Figure 3b). She indicated that there was less charge distinction than what is commonly illustrated in textbooks. This explanation indicated another instance where an instructor lost

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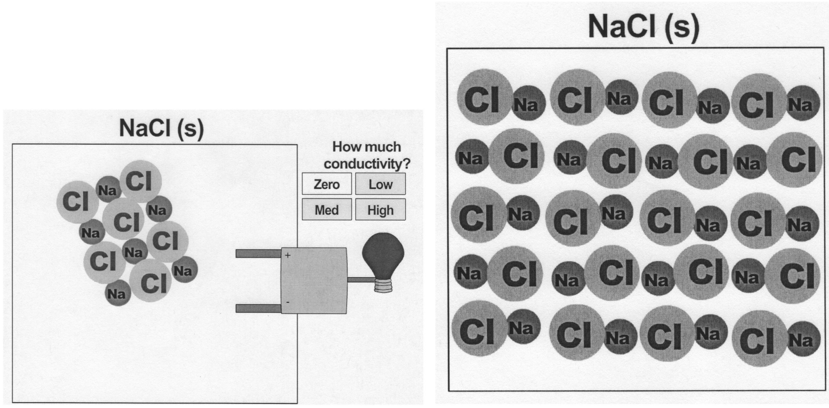
sight of representing a student's perspective and represented his/her expertise instead.



(a) (b)

Figure 3. (a) Instructor A's construction of NaCl (s) with a distinct rectangular shape. (b) Instructor C's lattice of NaCl(s) comprised of neutral atom pairs.

Another interesting difference noticed in instructors' pictures was the amount of space placed between the ions or atoms in the lattice. Four instructors showed some distance between the ions, but reasons for doing so varied. Instructor D indicated that this was a more accurate way to represent the proximity of ions in the lattice, indicating his understanding of ionic structure was not necessarily what he believed a student would convey. Instructor X confessed that it was unintentional, "it just happened." Instructor C noticed that while using molecules to construct her lattice helped her de-emphasize charges, she also realized that it created row-like appearances that she did not intend to construct. She indicated that there would be more equal distribution of space between the atoms in the lattice.

All of the instructors indicated that students should recognize that due to the lattice arrangement, ions would be immobile and would not be affected by introducing a conductivity tester into the sample. Thus, "good" students would recognize that solid sodium chloride would not conduct.

Aqueous Sodium Chloride after a Conductivity Tester Was Introduced

The most noticeable differences observed in the instructors' constructed pictures of aqueous sodium chloride were the number of ions used to represent the aqueous sample, presence of solvent water molecules, and whether hydration spheres or ion-dipole forces were represented between water molecules and ions (Table 1). All instructors represented a one to one ratio of sodium ions to chloride ions in their pictures, but the complexity of their depictions varied (Figure 4). The majority of the instructors (five) constructed pictures where at least two or sometimes three of each ion were represented, making their pictures seem more complicated than the pictures made by the four instructors showing fewer ions.

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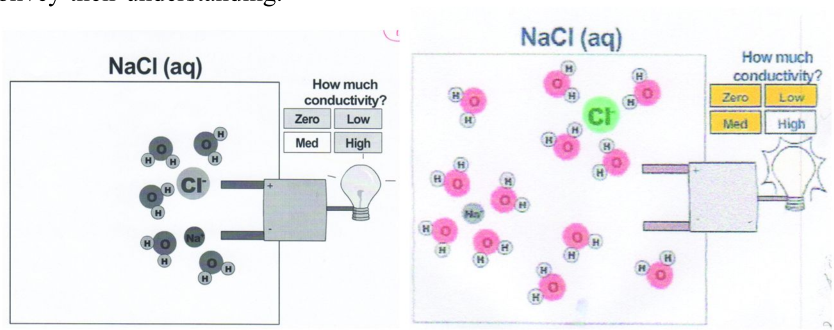
Typically, instructors who represented two or three of each ion tried to convey that while the formula of the compound implied the correct ratio of ions, there were multiples of the ratio in the solution. One reason instructors chose to represent one of each ion was because it better represented the number of ions in a dilute sample; however, another reason given was that it was sufficient for students to convey their understanding.



(a) (b)

Figure 4. (a) Instructor F's construction of NaCl(aq) being tested for conductivity. (b) Instructor D's construction of the same event.

Most (six) of the instructors represented ion-dipole intermolecular forces in the form of hydration spheres in their aqueous salt depictions. Only three instructors, two of which were current general chemistry instructors, represented the ions mixed with water molecules, but no intermolecular forces of attraction. Their rationale was that intermolecular forces were covered late in the first semester, thus they did not expect students to recall or represent it near the beginning of the semester. Most of the instructors indicated that ions would move toward the electrodes and all nine instructors felt students would recognize that aqueous sodium chloride conducted. However, three instructors expressed that aqueous sodium chloride would conduct at a medium level because the concentration was not specified and medium seemed like a more logical choice for a student.

Phase 2: Analysis of Three General Chemistry Instructors' Pictures and Interviews

As mentioned previously, three of the nine professors (identified by the letters X, Y and Z) were currently teaching Introductory Chemistry 1A at the time of the study or had just taught it the semester prior to the study. Analysis of interviews with these instructors revealed richness in their oral explanations, because they drew upon relevant teaching experiences and interactions with students when they conceptualized how general chemistry students would respond to the electronic worksheet exercises. In addition, since the goal of the study was to design visualizations for a general chemistry audience, it was important to thoroughly investigate features highlighted by general chemistry instructors. As a result, the

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interviews and constructed pictures of these three professors were the focus of this second phase of analysis, and this section demonstrates how their pictures and oral explanations were used in the design of visualizations.

Profiles of Three General Chemistry Professors

The atomic level pictures that were constructed by three general chemistry instructors revealed that they fell into two different categories: Simplistic and complex portrayals. They had different expectations of what a student should be able to convey through pictures when explaining the nature of a substance and its ability to conduct.

Dr. Y and Dr. Z were professors who favored simplistic representations for their general chemistry audience. Dr. Z provided a rationale for her pictures:

> *I teach a course (general chemistry) in which I lie. I lie, and another professor teaches the course tries not to lie, and I can see the beauty of that as a chemist, but students feel utterly overwhelmed with the minutia, and so I usually tell them the first day. We are lying! This is a general chemistry course. We are doing introductions. We are making things black and white, and we are not doing all of the shades of gray. Shades of gray starts in second semester.*

Dr. Z was very connected to her students and had strong beliefs about what they could handle in terms of atomic level details. Similarly, Dr. Y constructed pictures that were also very simplistic. Although he did not state his rationale as boldly as Dr. Z, he indicated that he was more inclined to focus on symbolic aspects of general chemistry. He did not often include atomic level details in his lectures. He chose to portray his own drawings in a symbolic format, using element symbols over particle shapes to emphasize connection to equations, an area that he recognized as being very difficult for students to understand. Both Dr. Z and Dr. Y provided insights into the minimal characteristics necessary to portray in the animations.

Alternatively, Dr. X favored complex, highly detailed representations. He stated,

> *I think I've always been visual in picturing it (atomic level), but to communicate that aspect of how I perceived and to formalize it in the modeling process and furthermore to connect to other models is a personal goal... Getting students to do the modeling is extremely important.*

Dr. X was the only instructor to report that he had experience designing atomic level animations. He also designed handouts for his course that expressed great atomic level detail. As a result, Dr. X considered many different ways to represent the atomic level pictures he was assigned to construct in the study. Specifically, he was very concerned with how color should be used to emphasize details, as well as how size and shape should be illustrated. His work, being more complex than the work of the other two instructors, helped inform ways to construct visualizations that modeled greater detail and accuracy.

Segment 1 - Distilled Water

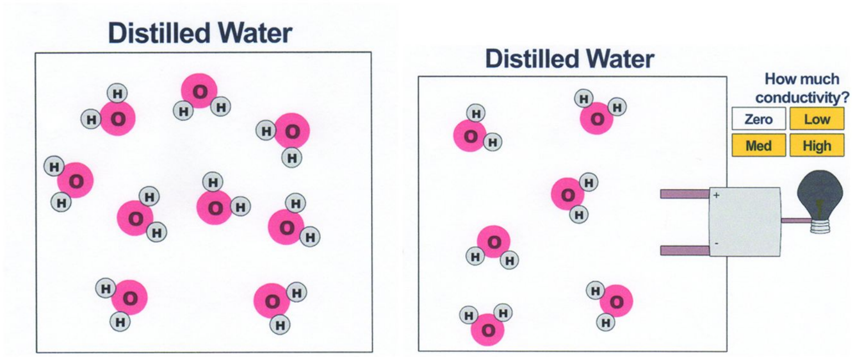
Dr. Z's pure water depiction was the most simplistic of the instructors. (Figure 5a) She represented nine water molecules separated by fairly large distances to show that intermolecular forces were not characterized. Since an intermolecular forces lab is given during the third week of first semester general chemistry at this institution, Dr. Z felt that intermolecular forces would not be covered prior to students using the tools. As a result she deviated from the intended task, which was to construct how a student after a full semester of general chemistry would represent the systems. Dr. Z defended placing large spaces between the water molecules because she felt students would not know about dipole-dipole forces at the time of using the animations. She stated, "I mean, I could keep putting them in, but I thought after six or seven, I'm cool...but I didn't know if they would think they (the water molecules) are bonding together." When demonstrating how pure water would respond to a conductivity tester, she reduced her population of water molecules to six and indicated that the conductivity would be zero (Figure 5b). In addition, she expressed concern with the macroscopic tester portrayed in the click and drag tool. In Dr. Z's words,

> *I was wondering if I should try to fit something in the space between the electrodes. I also wondered if the students would try to put all of the negative ions here (next to the positive electrode) and all of the positive here (next to the negative electrode). I was tempted to put it there but I know they are not going to diffuse all there so what do I do now?*

Her insights revealed that the modeled conductivity tester was problematic because it mixed the size scales. It would be best to keep the macroscopic level distinct from the submicroscopic level, and in later versions of the click and drag tool, the conductivity tester was removed from the atomic level box.

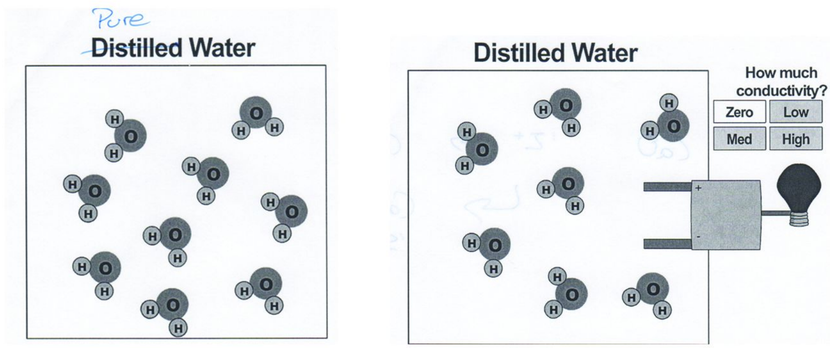
Dr. Y constructed similar pictures; however, in contrast to Dr. Z, he accounted for intermolecular forces (Figure 6a and 6b). He stated,

> *So I put these in trying to show hydrogens interacting with the oxygens and I rotated the molecules in order to do that. If this was the first time through and we hadn't discussed any intermolecular forces, I wouldn't expect students to be able to do that and I wouldn't mark them wrong. I would say just put some water molecules in there.*



(a) (b)

Figure 5. (a) Dr. Z's atomic level depiction of distilled water. (b) Dr. Z's atomic level depiction of distilled water tested for conductivity.



(a) (b)

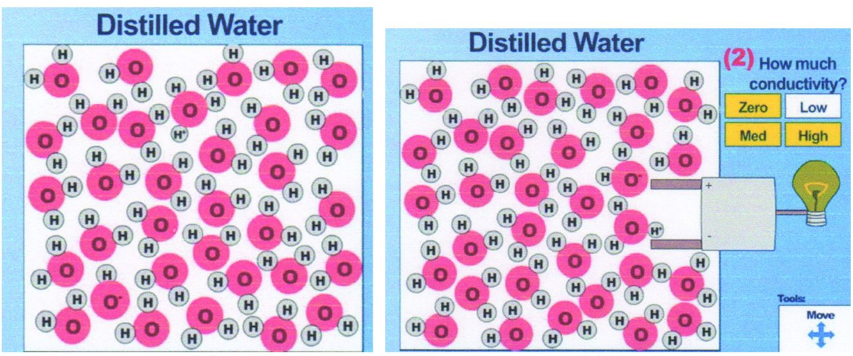
Figure 6. (a) Dr. Y's atomic level depiction of distilled water. On the printout, Dr. Y replaced "Distilled" with "Pure" in the description of water. (b) Dr. Y's atomic level depiction of distilled water tested for conductivity.

Dr. Y indicated that he would look to see whether students ionized the distilled water. "If they had a bunch of molecules and one or two ionized then I would say that's not entirely wrong. It's not necessarily the way I would cover it in CHEM 1A (general chemistry)." Dr. Y did not expect his students to illustrate the ions, and in his pictures he modeled that students would portray that pure water stayed intact as molecules and did not conduct electricity.

Dr. X constructed the most complex picture of distilled water of all three instructors. He accounted for some dissociation of water molecules into hydronium (top of Figure 7a) and hydroxide (lower left corner in Figure 7a), but he reflected on the difficulty associated with his portrayal. He stated,

> *For example, with one hydronium and one hydroxide ion we are teaching them that with 33 water molecules in there, that is three percent dissociated. I think that some of this is going to have to be done with hand waving. Maybe afterwards a critique that this is a limitation of the model and this is a distortion of the model and so you have to understand limitations and distortion.*

In fact, Dr. X recommended that there be a critique section at the end of every animation to encourage students to consider the limitations of the models. Dr. X constructed his picture of distilled water being tested for conductivity as weakly conducting (Figure 7b). Additionally, Dr. X recommended using the term pure water in place of distilled water as a good alternative, since many students may not understand what distilled means. Other instructors, including Dr. Y, similarly agreed that pure water would be an easier term for students to comprehend, and he recommended replacing the term distilled with pure, which is visible in his picture (Figure 2a).



(a) (b)

Figure 7. (a) Dr. X's atomic level depiction of distilled water. (b) Dr. X's atomic level depiction of distilled water tested for conductivity.

Distilled Water - Translation into an Animation

Kelly, Barrera and Mohamed (*23*) reported that the general chemistry students they studied tended to incorporate only one water molecule or at best a gaseous state representation of water when constructing pictures of aqueous salt solutions. Students felt it was unnecessary to include water molecules in aqueous solutions, because they did not think it to be important (*23*). As a result, even though some of the instructors did not include these concepts in their representations, this animation did include the water molecules because it was designed to help students assimilate the role of intermolecular forces and to remind them of the close proximity of molecules in liquid phase. The animation of liquid state pure water was also designed to accommodate instructors' insights (Figure 8). In order to account for the intermolecular forces that instructor Z anticipated students may not understand, partial charges were included to help students recognize that water molecules orient themselves to bring oppositely charged partial charges together. In addition, the narration provided an oral description of the process. The overall look of the animation was most similar to the representations of Dr. X as well as those from the other six instructors whose pictures are not all shown.

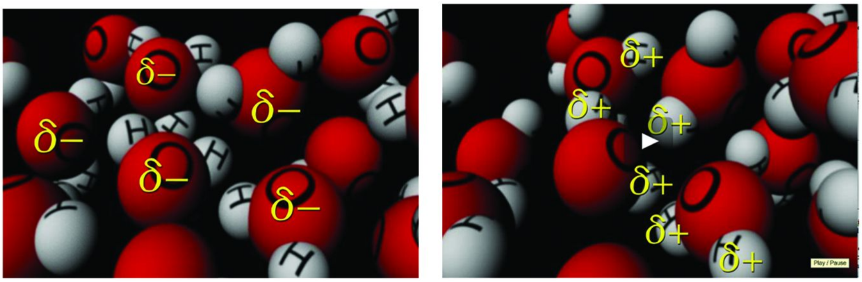


Figure 8. Still images from an animation of liquid state pure water showcasing partial charges and intermolecular forces of attraction. A limitation of the still images is that sometimes like charges are near each other temporarily; however, the brevity of this occurrence is lost in the still image above. Courtesy of Resa Kelly.

In order to address the best way to animate how pure water would respond to a conductivity tester, several of the nine experts recommended altering the macroscopic view of the tester in favor of a submicroscopic view. For example, Instructor F stated, “I don’t like these two prongs sticking in because we are on a molecular scale, and of course, this is not to scale” (Figure 2b). Instructor X added,

> *I could envision a nanoscale probe and maybe...allow more distance between the electrodes and then attaching it externally sort of magically. See this is the plane for nanoscale and this is the plane for macroscopic entities, and then that way you could make the electrodes atomically sized and show the atoms in the electrodes.*

Thus, the electrodes of the conductivity tester were atomically constituted as bronze looking spheres. The bronze color was chosen because it was the same color as the metal electrodes of a popular handheld conductivity tester used by students involved in the study, and the hope was that students would identify the atoms with the electrodes without having to label them. In addition, both electrodes were not represented in the same animation in order to illustrate that the distance between the electrodes was substantial at the atomic level. Since intermolecular forces were introduced in the animation of liquid state water, for consistency, the effect the electrodes had on the polar molecules was also illustrated. The animations were designed to show that the water molecules next to the electrodes would orient themselves to bring partially positive regions next to the negative electrode and vice versa. These molecules were highlighted to distinguish them from the bulk water. In addition, three different animations were developed to help scaffold the complexity of the pure water. To simplify the complex look, in one animation, a black backdrop was applied to help view the water molecules. (Figure 9a) In a second animation, the bulk water molecules were gray-scaled to help the viewer recognize the complexity of the liquid state yet still allow the viewer to focus on the surface level water molecules (in color) (Figure 9b). Finally, in the third most complex animation, the background water molecules were not gray scaled and the moving, complex nature of the liquid state was readily apparent (Figure 9c).

Segment 2 - Solid Sodium Chloride

The three general chemistry instructors had very similar atomic level models of solid sodium chloride. They all chose to represent two-dimensional crystal lattices with alternating positive and negative ions. Dr. Z purposefully constructed her lattice with ions that were somewhat separated to maintain consistency with her other pictures (Figure 10a). For example, her distilled water picture showed the water molecules to be relatively far apart. In the case of solid sodium chloride tested for conductivity, she did not intend to place the chloride ion next to the positive electrode or the sodium ion next to the negative electrode, and she indicated that it would not conduct (Figure 10b).

Dr. Y also represented a two-dimensional model of solid sodium chloride, and he felt it was important to illustrate the ratio of ions to be consistent with the formula. He stated, "It's a level of detail I wouldn't be too concerned with but it's a level of detail I can see a student doing and really worrying about the stoichiometry." He illustrated the lattice as slightly bigger than a unit cell, but he did not feel inclined to completely fill the box (Figure 11a). This view could be challenging for students, as they may believe that this was the quantity of ions in a grain of salt. Dr. Y expressed that solid sodium chloride would not conduct.

> *Now for the conductivity, it's not going to conduct because the ions are not mobile. I think the important point is that the solid is not conducting electricity. If you melt stuff, and you can certainly melt salts...it would conduct.*

He recommended showing how melting a salt would allow it to conduct (Figure 11b). He recommended illustrating potassium chloride or cesium iodide because they might have lower melting points making them easier to model as a demonstration or in the laboratory.

Dr. X took great pride in his 80-ion sample of solid sodium chloride, consisting of 40 chloride ions alternating with 40 sodium ions (Figure 12a). He expressed wanting a way to illustrate the unit cell, and felt it would be useful to seed the unit cell idea into the animation, but he also recognized that there were limitations to the model as true coordination numbers were not illustrated. He also noted that solid sodium chloride would not conduct. He reported in the interview that he purposefully tried to align the positive ion next to the negative electrode and the negative ion next to the positive electrode, although this is not readily apparent in his picture (Figure 12b). He asked the following question to a hypothetical student, "Why am I not getting conductivity? Because in every other instance where I have the ion I am implicating conductivity by having the ions touch the electrodes. Why isn't it happening here?" He felt that it was important for students to learn two things: It was the presence of ions and their mobility that caused conduction to occur. Even though ions were present, they were locked into place due to the strength of their electrostatic attraction, and they were unable to move to the electrodes to allow conduction to occur. Dr. X also recommended showing a video of a low melting salt to illustrate the ability of a molten salt to conduct.

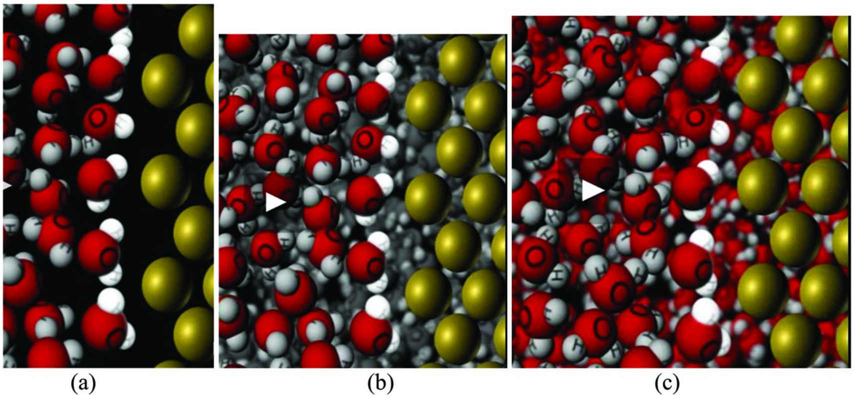


Figure 9. (a) Still image of pure water tested for conductivity with a less cluttered appearance of the bulk water. Only the water molecules in the first layer are shown. (b) Still image of pure water tested for conductivity with background water molecules gray scaled to reduce visual complexity, while water molecules in the first layer are in color. (c) Still image of the most complex view of pure water tested for conductivity. Courtesy of Resa Kelly. (see color insert)

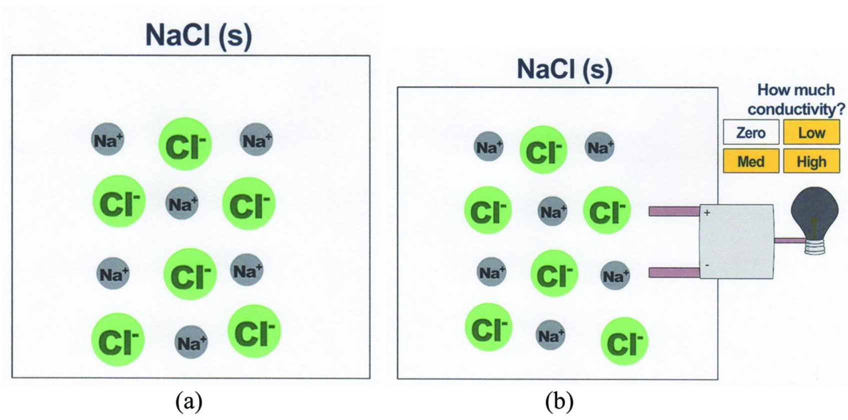


Figure 10. (a) Dr. Z's picture of atomic level solid sodium chloride. (b) Dr. Z's picture of solid sodium chloride tested for conductivity.

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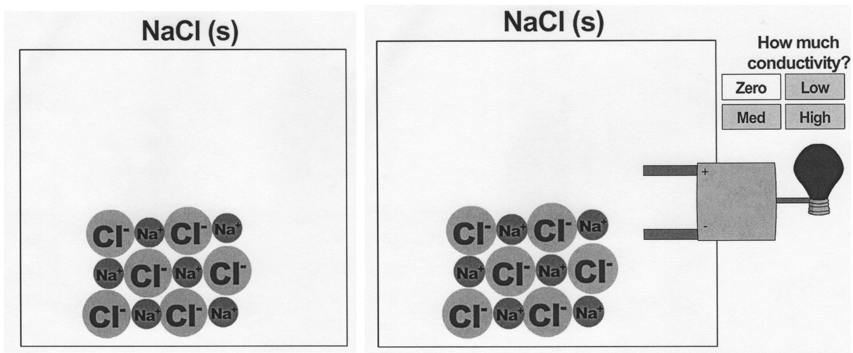
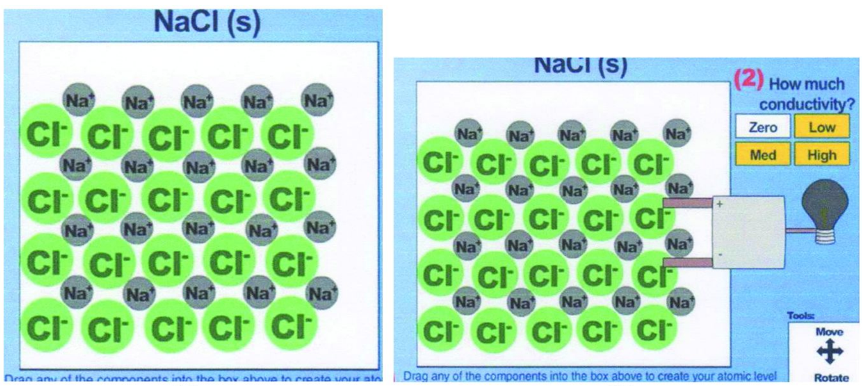


(a) (b)

Figure 11. (a) Dr. Y's picture of atomic level solid sodium chloride. (b) Dr. Y's picture of solid sodium chloride tested for conductivity.



(a) (b)

Figure 12. (a) Dr. X's picture of atomic level solid sodium chloride. (b) Dr. X's picture of solid sodium chloride tested for conductivity.

Solid Sodium Chloride - Translation into an Animation

The animations of solid sodium chloride begin with a two-dimensional view of the sodium chloride lattice before morphing into a three-dimensional view (Figure 13a & 13b) (*24*). This view was chosen because many of the nine instructors constructed similar two-dimensional representations. The benefit of the animation is that it is able to illustrate the vibrational movement of the ions as they reside in their lattice, yet are held in place by their electrostatic attractions.

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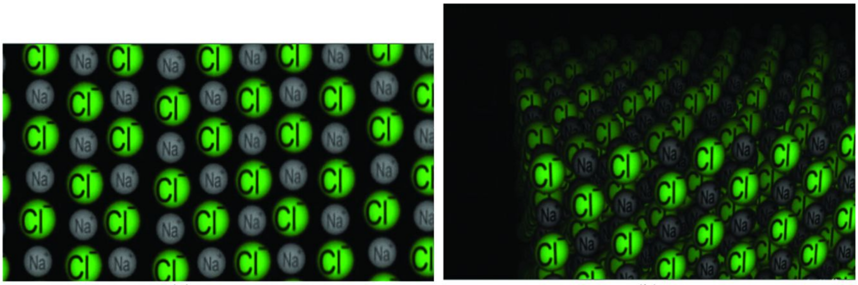
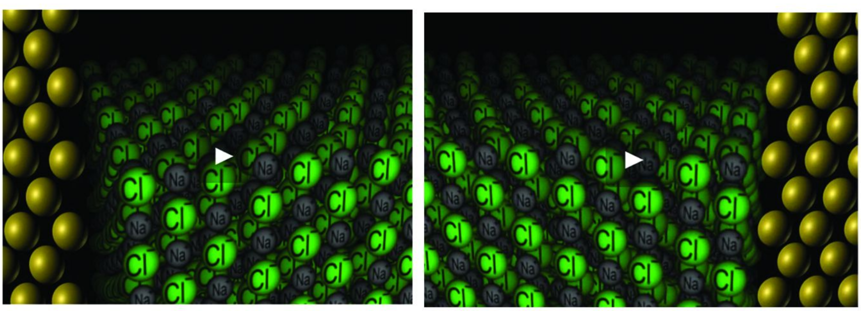


(a) (b)

Figure 13. (a) Still image picture of two-dimensional sodium chloride as it appears at the beginning of the animation. (b) Still image of a three-dimensional corner shot of the sodium chloride lattice at it appears in the animation. Reproduced from reference (23). Courtesy of Resa Kelly.

The animations of solid sodium chloride tested for conductivity also illustrated the vibrating motion of the ions in their lattice (Figure 14a & 14b) (*25*). The lack of movement toward the electrodes was explained by the accompanying narration, which stated that the electrical potential energy difference between the electrodes of the conductivity tester was not strong enough to dislodge the ions. Since there was no movement of ions toward the electrodes, there was no current and therefore no conductance. In order to illustrate the distance between the electrodes, the animation began at one electrode, then there was a sweep across the screen as if you were flying over the sodium chloride lattice until the other electrode was encountered. This process emphasized that at the atomic level there was considerable distance between the electrodes.



(a) (b)

Figure 14. (a) Still image picture of solid sodium chloride tested for conductivity next to an electrode. (b) Still image picture of solid sodium chloride tested for conductivity at the other electrode. Reproduced from reference (25). Courtesy of Resa Kelly.

As noted, Drs. X and Y recommended having a low melting ionic compound modeled so that students could see that the liquid state of an ionic compound allows the ions to move toward electrodes and conduct. As a result of this recommendation, video footage of sodium hydroxide being melted and tested for conductivity was made. The video will be used in an application section where the student may be guided through a scaffold of events. First, the student will be asked to predict whether molten sodium hydroxide will conduct. Second, he or she will be asked to select an atomic level picture that best represents the nature of this event and finally he or she will be asked to justify his or her prediction.

Segment 3 – Aqueous Sodium Chloride

To demonstrate the nature of a strong electrolyte, aqueous sodium chloride, Dr. Z separated the ions and primarily showed them mixed with water molecules (Figure 15). She emphasized that the most important detail was to make sure that the ratio of sodium ions to chloride ions was one-to-one to reinforce the connection to the formula. She thought it was important to show more than one of each species and the excess number of water molecules compared to the number of ions in an aqueous solution. She emphasized that she was not concerned about the location of the water molecules in terms of hydration spheres or how they would interact with each other.

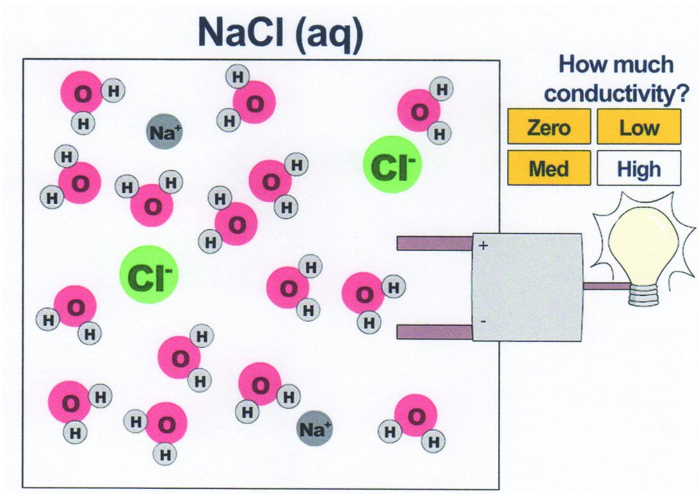


Figure 15. Dr. Z's picture of atomic level aqueous sodium chloride tested for conductivity.

When asked to demonstrate the nature of aqueous sodium chloride, Dr. Y was also concerned about the spacing between the ions. He tried to show how the hydrogen ends of water molecules were oriented toward the chloride ion and the

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oxygen end toward the sodium ion; however this was difficult to detect from his picture (Figure 16). During the interview, he emphasized that this was a level of detail he would expect students to understand if they had intermolecular forces. He acknowledged that he had done calculations to determine the arrangement of water molecules around a bromide ion and found it to be very different from how water molecules arranged around positively charged ions. He stated, "In the case of positive ions, the hydrogen ends of the water molecules were directed away from the positive ion and they were free to interact with other solvent water molecules." It is important to note that Dr. Y recognized this information as an additional layer of complexity that could be demonstrated for the students, but he did not represent this in his drawings. Another aspect that Dr. Y considered in making his picture was how to show the ions near the electrodes, but he pointed out that the reason it conducted was because it was not static. He expressed concern over showing the interaction between the ions and the electrodes. In Dr. Y's words:

> *Solvated electrodes and solvated ions are a very active area of research. The structures are not one hundred percent understood. It could be that what is making this all work is that this thing (the electrode) is polarizing all the water molecules around it. The polarization of the water molecules gives it a nice place for the electrons to go zipping through. It may be that the ions are not physically carrying the charge from one place to another, but disturbing the bulk (water) in such a way that it can carry a charge.*

In considering the nature of how aqueous sodium chloride conducts electricity, the general consensus of the nine professors interviewed was that the animations should avoid the interaction between the ions and the electrodes. In addition, Dr. Y thought it best to avoid depicting how the charge or the mobility of the ions affected conduction.

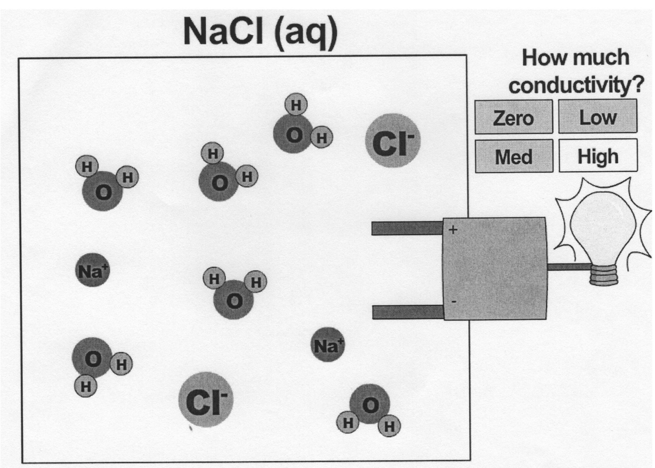

Figure 16. Dr. Y's picture of aqueous sodium chloride tested for conductivity.

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When approached with the same task, to construct a picture that represents how aqueous sodium chloride conducts electricity, Dr. X included three sodium ions and three chloride ions in his picture complete with spheres of hydration surrounding the ions and a comprehensive representation of the bulk water in the solvent (Figure 17). He indicated that his concentration would require some hand waving and that the animation should have a disclaimer that addressed the limitations of the model. In addition, he expressed concern about the size of the water molecules in relation to the size of the chloride ions. According to him, the water molecule should be around 300 picometers and the chloride was about 360 picometers. He felt that the size difference was too great as represented in the pictures. Thus, Dr. X did something none of the other instructors did. He provided a packet he used in his general chemistry course. In the packet he shared a picture that he found particularly useful (Figure 18). He described the picture as follows:

> *Teaching them about solution concentration...When I'm teaching them about solubility how we can represent this with words or a macroscopic picture or with a nanoscale model or symbolic model... so I am making the progression from the nanoscale to the macroscale. From the nanoscale to the ultimate simplicity of the modeling. Notice the difference in shading , see how I can show hydration, and that's what I would like to see in here are hydration spheres. If the two-dimensional equation is proportional to the 3-D what's its concentration? You can visualize concentration! It turns out we have 59 water molecules and 4 sodium chloride ion pairs so it's 3.5 M.*

Dr. X's interview illustrates how instructors have strong opinions about what they want to see in visualizations, and if these features are not represented Dr. X may be unlikely to use a visualization in place of his still image pictures. In addition, this interview illustrates the limitations of click and drag electronic worksheets. Sometimes the illustration options may not have the necessary features to capture the many intricate attributes people mentally construct in picturing atomic level details.

Aqueous Sodium Chloride -Translation into Animation

The atomic level animations showing conductivity of aqueous sodium chloride were developed in a manner that scaffolds from the more simplistic views (Figures 19a & 19b) (*26*) that were observed in the work of Dr. Y and Dr. Z to the more complex views reflected in the work of Dr. X (Figures 20a & 20b) (*27–29*). In simplistic representations, less solvent water molecules were depicted to allow the ion to be more visible. The concern is that this kind of representation could reinforce an incorrect view of the liquid state of solvent water. However, when the animation is shown in series from simple to complex, beginning with a view that is on par with the way students represent aqueous states may help students to focus on the movement of the ions toward the electrodes which is the most important feature of the animation. Building toward the complex view may help students to process the additional layers of complexity. The middle layer of complexity attempts to gray scale the meticulous details of the background solvent to help students retain their focus on the movement of ions to the electrode, while the final layer of complexity demonstrates the complex solvent environment through which the ions meander as they are drawn toward the electrode. Unfortunately, the animation artists assigned to create these visualizations were unable to vary the shading as requested by Dr. X in his sample picture, instead the artists softly illuminated the hydration spheres surrounding the ions to make them easier to track.

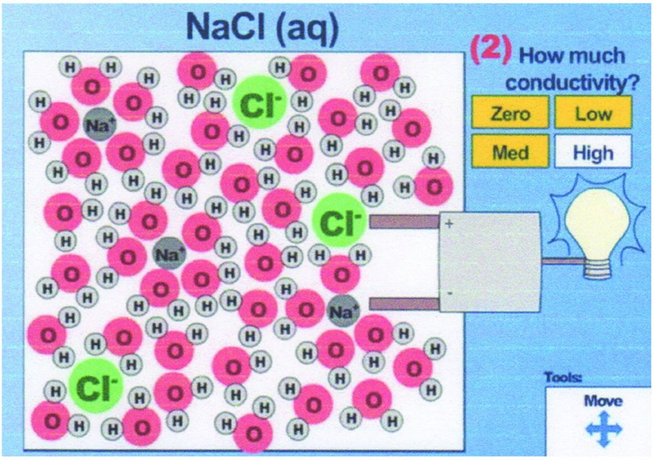


Figure 17. Dr. X's picture of aqueous sodium chloride tested for conductivity.

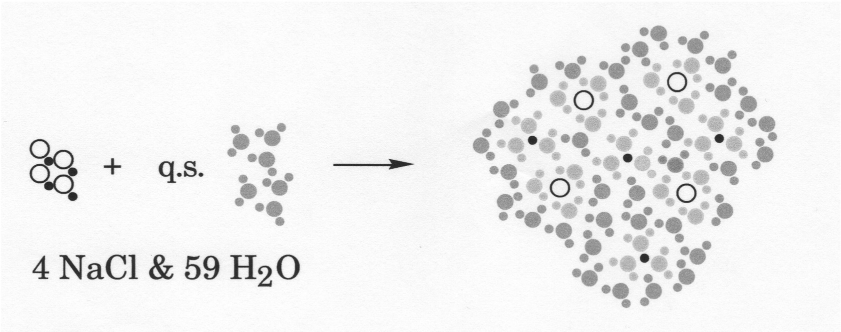
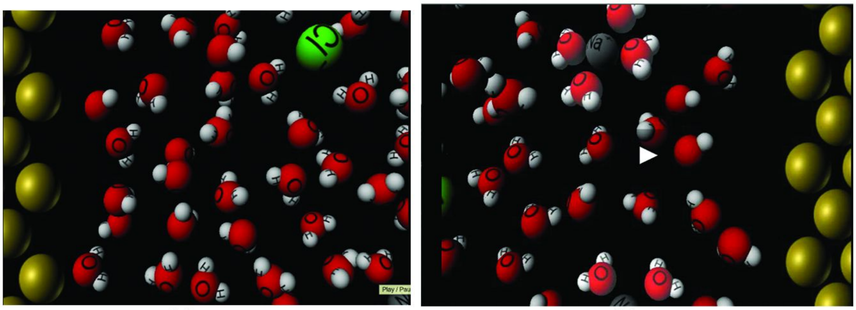
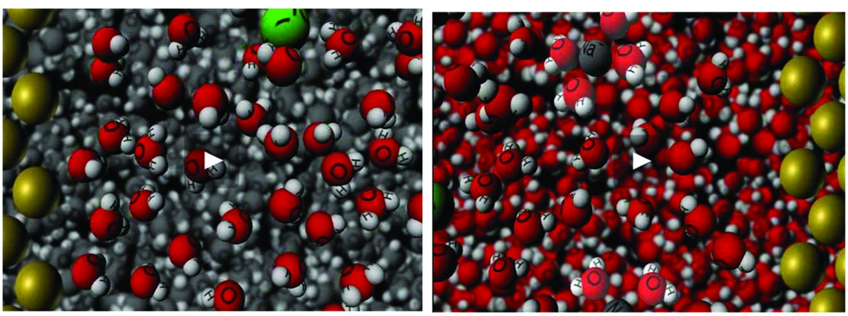


Figure 18. Dr. X's sample picture that he titled "Modeling Molarity: Physical to Mathematical (Assume 2-D model accurately reflects true 3-D solution)."



(a) (b)

Figure 19. (a) Still image from an animation of aqueous sodium chloride showing migration of the chloride ion to the positive electrode. Water molecules were removed to help students better see the chloride ion. (b) Still image from an animation showing conduction of aqueous sodium chloride as sodium moves toward the negative electrode. Water molecules were removed to help students better see the sodium ion. Reproduced from reference (26). Courtesy of Resa Kelly.



(a) (b)

Figure 20. (a) Still image from an animation showing conduction of aqueous sodium chloride with emphasis on the chloride ion migrating to the positive electrode. Background water molecules are included, but most are gray scaled to help the ions and superficial water molecules pop out for student viewing (27). (b) Still image from an animation of conduction of aqueous sodium chloride focusing on the migration of the sodium ion in a complex solvent background toward the negative electrode. Reproduced from reference (28). Courtesy of Resa Kelly. (see color insert)

Rationale Behind the Features General Chemistry Instructors Portrayed

When instructors were assigned to construct atomic level pictures that represented the features they hoped their best students would include if asked to do the task, it became clear that instructors drew upon their teaching experience, and their own understanding of the concepts, as well as their expectations of students' abilities for comprehension. The following excerpts from interviews with instructors X, Y and Z illustrate the instructors' rationale.

1. Examples demonstrating instructors' references to their teaching experience or pedagogical content knowledge:

> Instructor X: *For example, the Oklahoma state simulation for gases, I use that very effectively in lecture, but the first thing I do is tell them why I think it's realistic and why I think it's not realistic.*

> Instructor Y: *I just want them to understand that this dissociates into ions and "aq" means in a water solution. I'll mention there are waters of hydration [when I teach], but I won't go into great detail about what the structure is.*

> Instructor Z: *You could show a molten [state], you could show how you raise the temperature and it's now molten. We don't do that in lab anymore. We used to melt sodium hydroxide. We used to do it because it's one of the easier salts to melt, so they could melt it and put the electrode in and it would conduct.*

2. Examples where instructors refer to their own understanding of concepts:

> Instructor X: *We are not teaching the true coordination number because here we've got 4:4 coordination, whereas in sodium chloride it's 6:6. You don't want to teach them that this is what sodium chloride looks like, but this is just a mimic.*

> Instructor Y: *I noticed that I interpreted the hydrogen with a gray circle to be a hydrogen atom, and so I wouldn't have selected that because in my brain that was saying dissociating into neutral atoms, which is what it would do in the gas phase. Nothing in the gas phase dissociates into ions so it all dissociates into atoms. If you have a hydrogen chloride molecule in the gas phase and you zap it with a laser so that's going to dissociate. You are going to get a hydrogen atom and a chlorine atom.*

> Instructor Z: *I guess it could be medium [referring to conductivity of a sodium hydroxide solution], because in my head I am thinking how does the hydroxide...this is me, not the student, I've got sodium on both sides how does hydroxide compare to the mobility of the acetate [another anion]?*

3. Examples where instructors refer to their expectations of students' abilities:

> Instructor X: *Maybe they have had experience with pH in their high school chemistry and they realize that there are some residual ion components in there so they go ahead and include them. I'm not quite sure how the student is going to choose or not choose to put in ions.*

Instructor Y: *Here I tried to arrange it so that the hydrogens are organized around the ion, so that the oxygen end is pointed toward the silver and that's a level of detail I would expect students to understand if they had intermolecular forces.*

Instructor Z: *Don't say concentrated because they don't know and that's an interesting question, they don't understand that it is a relative thing. So they come from high school telling me if it's below one molar, it's dilute, above one molar, it's concentrated. And I talk to high school AP teachers and that's what the books tell them. At least they know that higher molarity is more concentrated, but it's still a relative thing, who's more dilute, who is more concentrated?*

Evidence from interviews indicated that instructors thought about how their students learned over the course of the semester. In essence, they illustrated their hypothesis of how students' learning progresses. Learning progressions have been described as the successively more sophisticated ways students' understanding of core scientific concepts and explanations develop over time (*30*, *31*). Although unfamiliar with learning progressions, which are based on research about how students' learning actually progresses, these instructors shared their logical analysis of how student understanding develops based on their personal experiences in teaching.

Building the Context – Developing Electronic Learning Tools

The majority of this paper has been focused on how the atomic level animations were created. In this section, the focus shifts to examine how to present the animations to foster learning, because animations shown in isolation can be difficult for students to understand. Teichert, Tien, Anthony and Rickey report that that there is a specific connection between students' understanding of conductivity context and activation of students' molecular-level ideas about separated ions in solution (*32*). In order to create context for the animations and help students to build connections between the macroscopic and atomic level representations, the animations are embedded in a tutorial framework. This framework is referred to as an electronic learning tool (ELT). The design of the ELT is scaffolded to reflect a learning cycle approach, in that it consists of three components: Exploration, concept development and concept application. In the exploration section, a cartoon character acting as a tutor introduces video clips of demonstrations where solid sodium chloride and pure water, separately, do not conduct electricity (*33*). However, when the two substances are mixed together, the resulting aqueous solution is found to conduct electricity. By introducing this laboratory demonstration as a scaffolding step, students are invited to ponder what is happening at the atomic level to account for these different conductivity results. Multiple representations allow students to better understand connections between the various types of representations of a phenomenon and helps students integrate ideas that each of these representations provokes (*34*).

After students complete the exploration section, they are asked to complete two electronic worksheet activities similar to those completed by the instructors during this study. The activities are used to assess students' prior knowledge of the atomic level details of solid sodium chloride and aqueous sodium chloride tested for conductivity. Completion of the worksheets allows students the ability to access atomic level animations created from the research to determine why some substances conduct while others do not. Thus students will watch animations of pure water, solid sodium chloride and aqueous sodium chloride in the absence and presence of a conductivity tester. Once the students view all of the animations they will be asked to once again use the electronic worksheets to construct their conceptual understanding of solid and aqueous sodium chloride tested for conductivity. They will be shown the pictures they constructed initially, and they will be asked to describe any misconceptions they feel they had before viewing the animations. They will also be asked to describe the changes, if any, they made to their new pictures to reflect their current conceptions. This allows the students to reflect on what they have learned from viewing the animations.

In the concept development section, atomic level animations are introduced through a series of tutorials led by a cartoon character. These segments address: How a conductivity tester works, the electrolytic behavior of acids, the conductivity of acetic acid, and symbolic representations of strong electrolytes and weak electrolytes (*35–38*). In the tutorials, Dr. Ann Ion, teaches in a progression that shows simple key features and builds to include more complex details. For example, in the tutorial on the electrolytic behavior of acids, Dr. Ann Ion begins with a very simplistic still image model of separated hydrogen and chloride ions on her white board to allow students to focus on the key feature of separated ions (Figure 21). As the tutorial progresses, the still image models take on an additional layer of complexity showing hydrated ions (Figure 22). Finally an animation is introduced to illustrate moving hydrated ions in a very detailed network of moving solvent water molecules. Narration by Dr. Ann Ion helps clarify what the viewer is seeing and highlighting techniques are also used to scaffold the process.

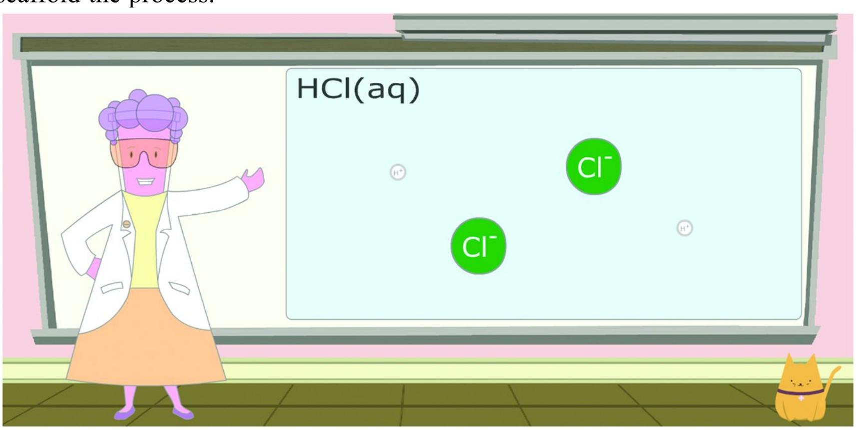


Figure 21. A still image picture of Dr. Ann Ion presenting a very simple representation of hydrochloric acid. Courtesy of Resa Kelly.

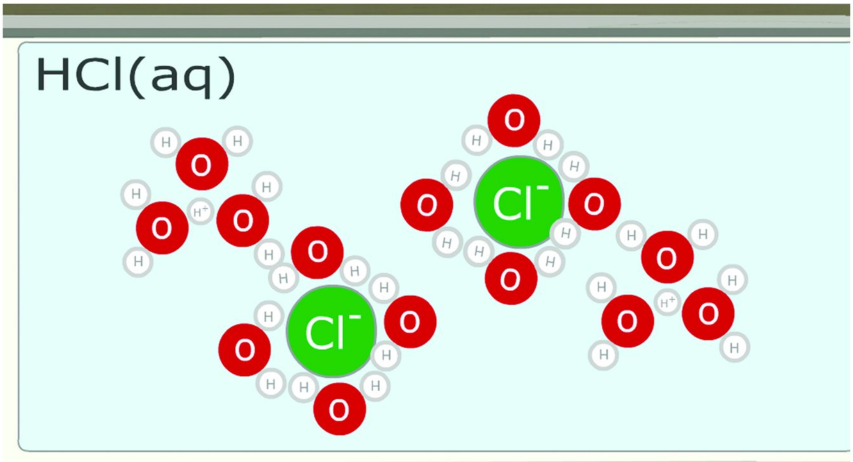


Figure 22. A more complex still image from the tutorial on the electrolytic behavior of acids. Courtesy of Resa Kelly.

Studies indicate that beginning general chemistry students have a limited understanding of the molecular and electrolytic behavior of strong electrolytes, weak electrolytes and non-electrolytes (*32*, *39–43*)). Many students will express only the simple whole number ratio of ions when constructing atomic level pictures. Teichert at al. (*32*) concluded that very few students were able to express correct molecular-level ideas regarding ionic compounds and molecules dissolved in water; however, they indicated that context may activate specific molecular-level ideas and lead to improved performance.

The animations and tutorials, from which the still image pictures in this paper were captured, are available for viewing on YouTube, but the ELT framework that will house the animations and tutorials is still under development (*24*, *25*, *35–38*). One section that we are currently developing is the application section. In the application section a scaffold will be developed that requires students to first predict whether a substance will conduct given only the formula of the substance. Then the students will be asked to select an atomic level picture that best represents their predictions. Finally students will be given evidence of the conductivity events in the form of video clips, and the student will then be allowed to change their selected pictorial accounts to fit the evidence that they witness.

Addressing Model Limitations

In order to address limitations of the atomic level animations, a cartoon cat, named "Cat Ion" was introduced in the tutorial segments to make announcements or point out places where liberties were taken in the design of the atomic level. For example, in one of the announcements the cat mentions that chemists prefer to represent the dissociated hydrogen ions that are shown in the tutorials as hydronium ions. Some students are unfamiliar with hydronium ions and as a

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result we chose to depict hydrogen as free ions in solution. In another scenario, an oral announcement was made that two 0.1 M solutions were represented for simplicity as four molecules. By having these cues some of the "hand waving" issues that Dr. X referred to previously were acknowledged.

Discussion

The goal of this study was to reveal a coarse level of key atomic level details central to understanding how substances respond to a conductivity tester and how the system should evolve to include more complexities, which reflects a knowledge-in-pieces approach (*18*, *19*). The results of this investigation illustrate how instructors who teach general chemistry can have very different expectations for the kinds of details they want their students to be able to convey to show mastery of atomic level details. Designers must recognize that these different levels of complexities can be useful for designing scaffolds of the concepts being animated, and if these different levels are represented in a visualization, it will have wider appeal to both instructors and students. In this study, it was shown that the instructors differed primarily on how best to represent the liquid state of pure water when it was alone and when it was acting as solvent. Instructor X showed a very detailed perspective with many water molecules while Instructors Y and Z were happy if the water molecules were present, but they were less concerned about the intermolecular forces being perfectly displayed. The presence of water can make it very challenging to notice the more important details of separated ions and how the ions migrate toward their respective electrodes (*2*, *21*, *44*). However, if water is left out of pictures, students may not recognize the importance of the water molecules in the migration of ions toward electrodes or worse they may not recognize that water is present.

The still image pictures from the animations and tutorials show how instructors' insights can inform the design of animation scaffolds where the level of complexity increases with each animation. However, a limitation of this study is that it does not share the students' perspective. Understanding the kinds of pictures students construct to explain their atomic level understanding provides a starting point from which to bridge connections to their understanding. Kelly (*45*) noted that when a student did not know how to picture the atomic level, presenting the student with an accurately detailed animation where many ions and water molecules were shown was overwhelming and rendered the accurate animations useless. Thus, finding ways to bridge how students with simplistic views are able to connect to the content presented in the atomic level animations is important to help learners make progress. To quote Tasker and Dalton, "We need to direct our students' attention to their key features, avoid overloading working memory, and promote meaningful integration with prior knowledge" (*21*).

An animation scaffold consisting of a sequence of animations ranging from simple to complex is often desirable, but what level of detail and accuracy should the continuum support? Some instructors feel it is important to always present students with the most accurate and theoretically sound representations possible. For example, consider the latest theory for depicting the electrolytic behavior of an acidic solution. Tuckerman, Marx, and Parrinello (*46*) recently revealed insight into how protons are transported in aqueous solution. The research describes the detailed importance of the complex solvent network surrounding hydronium ions. For example, breaking a hydrogen bond between two water molecules that surround a hydronium ion causes a proton associated with this hydronium to transfer to the closest water molecule of the two that broke apart. The question is: Should we present this information to a student in first semester general chemistry?

General chemistry students have difficulty recognizing how hydrogen ions react with water molecules to form hydronium ions. Some students rarely include solvent water in their drawings and do not consider its importance (*4*, *23*, *32*). Other students taught primarily with symbols and equations fail to visualize atomic level detail (*23*). If one were to show an animation of proton transport mechanism to a first semester general chemistry student, the student might be so distracted by solvent water that proton transport would go unnoticed. However, if the process were scaffolded, perhaps it would be possible to teach the details of proton transport theory. The question is whether this information is relevant to our general chemistry student audience as they progress through the general chemistry curriculum? Should we try to teach about this one complex process or be satisfied with getting the student to recognize that a solution that conducts is able to do so because ions are present and those ions are mobile? From this research, it seems that the nine instructors that participated would be satisfied with the later and would be willing to let the chemistry students who progress to upper division courses tackle the complex process of proton transport.

Conclusions

Segmented and scaffolded atomic level animations designed based on professors' instructional experience with general chemistry students can provide the needed bridge to move students from underdeveloped atomic level understanding to embrace a more detailed and coherent atomic level view. If students are first provided with a picture or animation that fits with how they imagine the complexity so that they are able to discern how their understanding compares to the animation before a more complicated view is presented, learning may be enhanced. In addition, instructors may be more inclined to use the animations if they can visibly see a connection to their pedagogical views.

Future research will explore the kinds of key features and alternate conceptions general chemistry students incorporate in their atomic level depictions of substances tested for conductivity when they are presented with a click and drag tool for making atomic level pictures. In addition, the research will investigate how students change or correct their atomic level pictures after viewing atomic level animations, designed from this study. By studying how students with poor conceptual understanding are affected by the animations, conceptual bridges will be developed to help these students better assimilate the information they encounter in the detailed atomic level animations.

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Chapter 10

Use of an Interactive Computer-Simulated Experiment To Enhance Students' Mental Models of Hydrogen Bonding Phenomena

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An interactive computer simulation was created to enhance students' conceptual understanding of hydrogen bonding in water. In a second-semester general chemistry course, 116 participants were categorized with respect to their levels of prior knowledge (PK) of the chemistry phenomena before they interacted with the simulation. This mixed-method study examined the effectiveness of the simulation upon their content knowledge (PK), pre-and post-intervention mental models (MM), and their perceptions. ANOVA Repeated Measures revealed that the simulation helped students improve their MMs (increased number of scientific conceptions) and reduce their misconceptions at both the observable (macroscopic) and molecular (submicroscopic) levels. Regardless of their PK level (low-, mid-, high-), there were no differences in their pre-to-post MM gains. Perceptions towards the simulation were positive for most students. These findings suggest that a well-designed simulation can reduce cognitive load while enhancing meaningful conceptual understanding (i.e. mental models).

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Introduction

Meaningful Chemistry Learning

People learning science should make use of their existing conceptual framework, including both concepts and relations, in order to understand their sensory experiences**.** A main goal of teaching and learning science is to promote meaningful learning rather than learning by rote (*1*). Ideally, students should be able to acquire meaningful conceptual knowledge by connecting newly acquired knowledge to their existing cognitive structures (i.e. their prior knowledge). This constructivist mode of learning can generate a deep understanding that allows students to interpret their learning environments and to create new ideas that can help them make sense of these environments (*2*, *3*). Thus, their conceptual framework can be revised (*4–6*), which allows them to make sense of additional experiences (*7*). In this research study, the goal was to help students develop a meaningful understanding of hydrogen bonding in aqueous solutions.

In contrast to the goal of promoting meaningful learning, as described above, chemistry instruction often induces students to learn isolated facts and algorithms, which are difficult to connect in meaningful ways (*4*, *8*, *9*). Thus, when engaged in rote learning, students cannot extend their knowledge beyond the limits of the classroom into their real lives (*2*, *10*, *11*). Also, it can result in many students holding prevalent chemistry misconceptions (*12*), which interfere with learning by distorting the new concept (*13–15*).

To overcome 'rote learning', instructional strategies, e.g. context-based learning, have been developed to encourage meaningful learning in chemistry courses by using learning activities connected to everyday life phenomena (*16–19*). In this study, we designed dynamic visualizations that refer to everyday phenomena—water droplets on different surfaces— to help students overcome the obstacles they face with the abstract concepts of intermolecular attractions and temperature effects on these attractions in aqueous solutions.

Hydrogen bonding is an important intermolecular attractive force that students need to understand in terms of its chemistry concepts and its many applications (*20–22*). These concepts are abstract, difficult, and complex (*23*, *24*), and they can illustrate the interplay between macro- and submicroscopic representation levels of chemistry knowledge (*25*, *26*). However, many students have misconceptions regarding these levels (*27–29*). Thus, they have great difficulty in transferring their understanding to the corresponding real world phenomena (*10*, *23*, *27*, *30*, *31*). These factors create barriers for meaningful learning that can adversely influence the learning of other chemical concepts (*31*).

For science educators, visual representation technologies have become increasingly important (*32*). Computer animations and simulations can provide a high quality of visual learning by imitating dynamic systems of interacting objects while simplifying theoretical models of real world phenomena. Researchers have found that computer animations and simulations can either reduce or induce students' misconceptions (*33–36*). Simulations can also help students improve their scientific process skills (*37*), acquire more qualitative knowledge (*38*, *39*), develop a more coherent understanding of the concepts (*40*, *41*) and facilitate the construction of mental models (*42–44*).

Mental Models, Understanding and Chemical Representations

The Constructivist theory states that understanding is not something that can be transmitted from teacher to student or from student to student. To understand the world, students must acquire a comprehension of concepts by themselves, and this process requires the construction of mental models in their minds. Although this conceptual process is relatively easy for chemists—who by definition are 'experts'—it is difficult for students who are 'novices'. Experts have highly organized mental structures, called *schemas*, that allow them to select, categorize and make sense of incoming information and their experiences (*45*, *46*). These schemas are stored in and retrieved from long-term memory. Thus, experts can easily acquire new information because they can relate it to the appropriate schema in their minds (*45*). A schema contains only 'what' is known; however, it does not include 'how' it should be used in a particular situation. Conversely, a *mental model* combines a schema with a process of manipulating the information in the schema (*47*). Thus, experts can use their relevant mental models to solve complex problems because their models are more abstract, elaborate, stable, interconnected, and integrative (*46*, *48*, *49*) than those of novices.

Mental models allow students to go beyond a surface understanding of the presented information and to build deeper comprehension of concepts in a domain, e.g. chemistry (*48*). These models are always under construction while being based on existing and newly acquired knowledge, ideas, conceptions, and experiences (*48*). During the learning process, the development of mental models varies as students' experiences increase, and superior performances are reflected in how well they develop their own mental models (*48*). This wide variety of previous experiences results in many different levels of student conceptual understanding (*49–52*). When performing complex tasks in a given domain (e.g. chemistry), students who possess highly developed mental models can make sense of their experiences, understand a phenomenon and its underlying science principle, and produce more accurate problem-solving results (*48*, *51–56*).

Conceptual understanding in chemistry requires the ability to use multiple representations as illustrated by Johnstone's three levels of representing chemical knowledge (*57*, *58*). Lectures tend to emphasize *symbolic representations*, (e.g. chemical equations or mathematical manipulations); whereas, the laboratory focuses on *macroscopic representations,* which involves planning, making and recording observations of chemical phenomena (*59*, *60*). The third one is the *submicroscopic level* (also called the molecular or particulate level) (*57*, *58*, *61*, *62*), where atoms, ions and molecules are represented as icons (i.e. circles of different sizes and colors to represent different chemical species). When students possess inadequate or inaccurate mental models at the molecular level, they often have great difficulties understanding concepts and thus they express many misconceptions (*6*, *51*, *61*, *62*). When students use submicroscopic representations for a chemical process, they should be encouraged to recognize, draw and explain the correct numbers and shapes of these icons, which, in turn, can serve as a visualization tool for learning abstract concepts, provide a more complete picture of the chemical process, and lead to a deeper conceptual understanding (*49*, *52*, *63–68*).

Chemists, as experts, can easily interconnect these three chemistry representation levels (i.e. macro-, submicroscopic, and symbolic), and their mental models are much more coherent and integrated than those of students (*68–71*), who often lack the requisite prior knowledge. Thus, Devetak and Glazar (*72*) developed a model of *interdependence of multiple representations* that shows the three levels as overlapping 'Venn diagrams' to account for the features of one representation being complementary to the corresponding features of the other two representations. Furthermore, they define the area of 'triple overlap' in the middle as being a *mental model* of the chemical phenomenon being studied. The pedagogic implication from this model is that visualization methods, such as animations and simulations, should be explicitly designed to support student development of a scientifically correct mental model. This student-generated model can then be used to interconnect a chemical phenomenon (e.g. lecture demonstration of the combustion of propane in air) with its symbolic (e.g. balanced chemical equation) and submicroscopic representation (e.g. visualizing a limiting reactant problem). Chemists, as experts, see all of these specific representations as different aspects of the same phenomenon; however, students often see these representations as three separate worlds that can only be memorized as separate entities.

Talanquer (*73*) based his *model of chemistry knowledge space* on an expansion of Johnstone's model (discussed above) to include *sensory experiences*, *visualizations* and *models* of chemical systems. His model is very useful in describing how learning progresses from misconceptions (i.e. pre-conceptions developed from past experiences) to the models that chemists, as experts, have developed "to describe, explain, and predict the properties and behavior of matter (p. 188)" as complex chemical systems. Thus, students' *prior knowledge* is an integral factor in determining how well and how rapidly they can maneuver from their experiences with chemical phenomena to the internalization of abstract models that allow them to understand chemical processes and concepts (*73*). In this research study, we essentially used this model to provide the instructional support for students to interact with simulations of hydrogen-bonding phenomena in aqueous solutions (i.e. shape and contact angle of water droplets), and to connect these macroscopic representations with the underlying submicroscopic representations of the intermolecular forces while illustrating the effects of temperature and type of surface (i.e. hydrophobic or hydrophilic) at both the macro- and submicroscopic levels of representation.

Multimedia Models and Prior Knowledge

When constructing mental models from multimedia visualizations of complex learning tasks, students benefit from support provided by the visualization software (*74*). As shown in Figure 1, students must process two types of information—verbal information from text or voice and visual information from pictures or diagrams. Schnotz and Bannert (*74*) clarified this distinction by calling the former type of information 'descriptive representation', which uses symbols to describe an object (*74*). They define pictorial information as a 'depictive representation', which allows students to 'see' the relations between

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visual objects without the use of abstract symbols. For example, an iconic sign for a water molecule is represented as $_oO_o$ (bond angle, 105°).

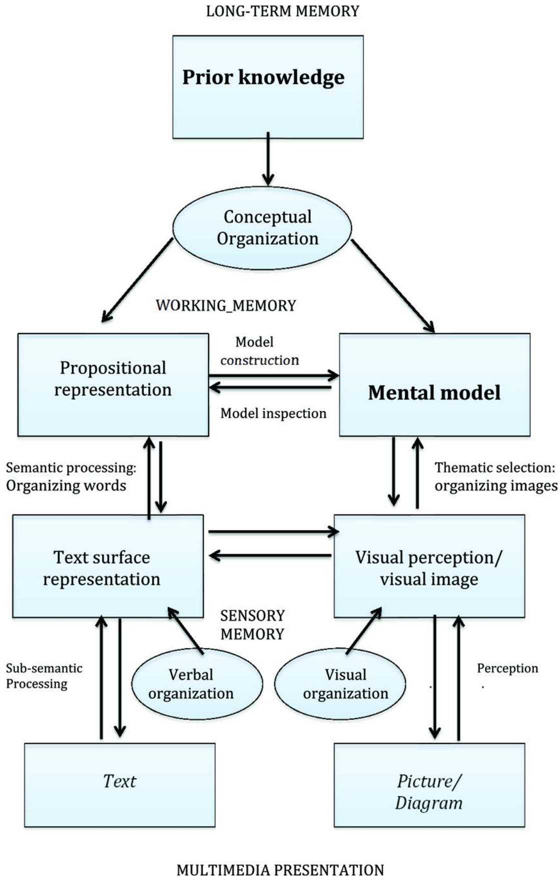

Figure 1. An Integrated, Cognitive Model of Multimedia Learning. Adapted from Schnotz & Bannert (74) & Mayer (76)

Next, the student must process this verbal and visual information on separated dual channels (*75*); that is, when they perceive an external text representation, it must be 'verbally organized;' meanwhile, the external visual representations, such as pictures or diagrams, must be visually organized to form imagery representations. Next, the verbally organized representations must be "semantically processed" to form the more abstract "propositional representations". Finally, to construct their "mental model", the student must integrate these propositional representations with those visual representations that have been thematically organized (*74*). Meanwhile, they must selectively focus only on the *relevant features* of each type of representation. Otherwise, they can be distracted if the images are perceptually salient (e.g. brightly colored solvent molecules) but not relevant to the underlying conceptual theme.

On the one hand, Mayer's cognitive theory (*76*) of multimedia learning differs from Schnotz and Bannert's (*74*) integrated model of text and pictures (see above section) in that Mayer includes the *prior knowledge* of the learner, which is activated from their long-term memory when the verbal and pictorial representations are integrated together (see Figure 1). On the other hand, Schnotz and Bannert's model (*74*) emphasizes that pictures can be "visualized in a variety of different ways." Thus, a specific visualization can either enhance or inhibit the structure of the mental model being constructed (*74*). That is, if *task-appropriate* pictures are used, then multimedia learning enhances mental model construction, while the use of *task-inappropriate* pictures can inhibit this construction process. When these two cognitive models are combined (see Figure 1), the learner's level of prior knowledge can interact with the appropriate visual representations.

With regard to developing viable mental models, students with higher levels of prior knowledge have larger 'chunks' of information in their working memory, which are more inclusive while allowing them to integrate representations (*54*, *77*) without much instructional guidance. Conversely, students with lower prior knowledge have smaller chunks in memory, which often results in cognitive overload; especially when faced with learning a complex task that requires them to connect multiple representations. Their lack of prior knowledge can result in their lack of ability to identify relevant structures in the multimedia visualization (*77*). They typically focus on only one representation—the one that is the most familiar or simplest (*68*). Furthermore, when they try to interconnect multiple representations, they tend to focus on the surface features (e.g. the brightly colored red and white spheres of the water molecules in the surrounding medium) because they are often unaware of the underlying relevant features (*68*). Overall, different levels of prior knowledge (PK) of chemistry can result in students using qualitatively different learning strategies. That is, students with low PK may devote much of their cognitive resources in trying to build mental connections, while those with high PK may be using the visual cues in the animation to link, integrate and elaborate upon these connections. Therefore, in this research study, students' level of prior knowledge of chemistry content in the simulation (i.e. hydrogen bonding in aqueous solutions) is used as an important factor to determine whether they can integrate the verbal and visual representations into coherent, scientifically correct mental models.

Several research studies have established that *prior knowledge* of a chemical phenomenon and its multiple representations (i.e. both verbal and visual) gives students the ability to solve complex problems, make decisions, understand abstract concepts, reduce their misconceptions, generate their own representations, and predict and explain the phenomenon at the molecular level (*6*, *78–80*). Also, numerous studies have reported that students' prior knowledge of the content determines which students can successfully learn from visualizations as opposed to those who cannot learn without the key features that provide explicit and relevant instructional support (*52*, *54*, *64*, *74*, *77*, *78*, *80–89*). Students with low prior knowledge need multimedia instruction that they perceive as more plausible and convincing than their prior knowledge (*52*, *90*). They also need to have abstract concepts clearly presented in order to link them as similar features across the visual and verbal representations being presented (*78*).

Visual representations must be presented in a manner that is appropriate to the learning task and thematically relevant to the underlying conceptual framework of the multimedia visualizations (*74*, *86*). Otherwise, the presented information may result in a cognitive overload in their short-term memory (*64*, *81*, *91*, *92*) while misdirecting their attention to salient perceptions that are irrelevant to the conceptual theme (*86*). These difficulties interfere with their ability to develop coherent mental models and a deep understanding of the presented material. Conversely, students with high prior knowledge are more likely to be able to mentally construct the necessary abstract concepts on their own (*78*). They are better able to actively process the relevant words and pictures, organize this information into coherent verbal and pictorial mental representations, and integrate these representations into a coherent mental model that includes their prior knowledge in this mental process. However, if the presented information contains visualizations that distract from the relevant concepts being presented, then even high prior knowledge learners may be hindered in their mental model constructions (*74*). In terms of this research study, the different levels of prior knowledge of the participants is a critical factor in accounting for the qualitatively different learning outcomes that the multimedia, constructivist instructional design of the hydrogen-bonding simulation (see next section) may have on the development of their mental models of these phenomena and their chemical representations.

Methodology

Purpose and Research Questions

The purpose of this mixed-method study was to design, use and evaluate the effect of the computer-simulation (CA-SIM) on students' conceptual understanding of hydrogen-bonding phenomena in water. All participants, who were enrolled in the second semester course in general chemistry, interacted with the CA-SIM. The appropriate statistical analyses were used to determine if students with different levels of prior knowledge (PK) learned differently from the CA-SIM environment as gauged by their chemistry knowledge and their mental models. Also, an established instrument (survey of perceptions) plus interviews with selected student volunteers (qualitative themes) were used to gauge their perceptions of the CA-SIM learning environment.

Specifically, this purpose was investigated using three research questions (RQ's):

RQ1: Did the CA-SIM intervention provide sufficient information such that students with less PK (Low- & Mid-PK) were able significantly narrow the gap in *content knowledge* with respect to those with greater PK (High-PK)?

RQ2: For students with different levels of PK, did the CA-SIM intervention significantly affect the pre- to post- changes in their *mental models* of the aqueous phenomena?

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RQ3: How did the CA-SIM intervention affect the perceptions of the learning experiences of students with different PK levels as gauged by a *perception questionnaire* and individual interviews conducted with selected students?

Participants

The college students, $N = 132$, were science majors enrolled in six lab sections of a second-semester course in general chemistry at a mid-sized state university in the western US. All students were informed of the nature of this research study, and the participants were 116 students who freely signed the IRB-approved consent forms and completed all activities in this study. Students who did not sign were not included in this study. Participants had just completed a laboratory experiment on intermolecular forces, which featured the following subtopics: cohesive and adhesive forces, effects on intermolecular forces, viscosity measurements, and enthalpy of fusion of water.

Instructional Materials: Design of CA-SIM

Design Rationale and Principles

The Contact Angle Simulation (CA-SIM) was the instructional material developed for and used in this study. It is an interactive computer-simulated experiment on aqueous hydrogen bonding and water contact angle, which is represented at both macroscopic and submicroscopic levels. The goal of CA-SIM was to engage students in a complex learning task in which they encountered and eliminated their misconceptions of hydrogen bonding, while constructing meaningful understandings of these phenomena. CA-SIM consisted of three sequential stages: *Introduction*—to prepare students, *Simulated Lab*—to engage students in decision-making and observations of simulated outcomes, and *Test Yourself*—to provide opportunities for self-assessment. The URL for CA-SIM (accessed on 20 Mar 2013): http://ednet.kku.ac.th/niwsri/simulation/hbond.swf

Constructivist-based design provides a rich context where meaning can be generated based on an individual's existing experiences and evolved conceptions (*93*, *94*). To further support student learning, instructional representations were designed to facilitate schema construction and reduce unnecessary cognitive load (*68*). For example, in all three stages of the CA-SIM, *scaffolding* provided opportunities for student interactivity while being supported by instructional guidance and illustrated by multiple representations of the aqueous phenomena. Three types of scaffolding (i.e. conceptual, procedural, & strategic scaffolds) were used to help students 'see": (a) the meaning of key concepts and their representations, (b) how to use the available software tools, and (c) identify what information is needed to guide their experiences (*91*, *95*). For example, as shown in Figure 2, the box-shaped "call outs" (#1 to 6, below) are designed to support student understanding of the procedure(s) to be used. Caption #1 shows the values selected for each parameter (i.e. temperature and contact angle); #2 shows the macroscopic view of the water droplet; and #3-5 show the molecular

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level with water molecules and the hydrogen bonds between them; and #6 shows the "slide" that students can use to select a new temperature and then observe its corresponding contact angle. Furthermore, instructional guidance was frequently incorporated into all three stages to help students stay focused on the concepts they were learning (*83*, *96*, *97*).

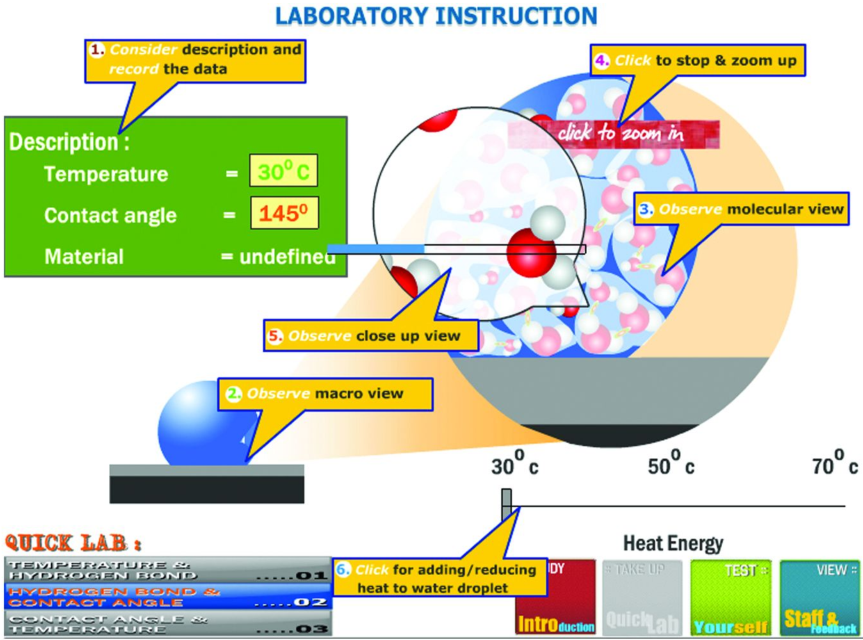

Figure 2. Screen shot from the CA-Sim visualization that shows instructional guidance in the form of "call-out" boxes #1 to 6 (see color insert)

The Construction of CA-SIM

After consulting with the first author, the second author developed a storyboard for the simulation. He used this feedback in the design and construction of the Macromedia Flash MX 2004 software. Design features that were incorporated ranged from basic elements (e.g. drawing graphics of atoms, molecules, and so on) to advanced elements (e.g. programming script on changing parameters and producing realistic motions). The first versions of CA-SIM were tested by three experts, one instructor and two graduate students, who examined both its chemistry content and its pedagogic effectiveness. The experts' suggestions were then incorporated into the subsequent versions in order to debug, edit and enhance its appearances. Also, the second author added examples of applications from daily life (e.g. hydrophobic property of waxing and coating), edited test questions and clarified test questions that required students to make decisions regarding the simulation parameters.

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Content Knowledge of CA-SIM

At the *macroscopic level,* the properties of liquid water provide indirect information about the intermolecular forces that exist among the water molecules. At this level, the term "wetting" describes a drop of water that spreads across a solid surface. The wetting behavior is determined by the contact angle formed at the liquid-solid surface. As the temperature increases, the droplet spreads out across the surface and the contact angle is reduced; vice versa for decreases in temperature. The hydrophobic/hydrophilic nature of the solid surface is also a factor in determining the resulting contact angle. Students learned about this factor during the Introduction stage of CA-SIM.

At the *molecular level* (or submicroscopic level), the contact angle of a water droplet on a solid surface is an indirect measure of fundamental molecular forces acting between liquid molecules and the solid surface that affect the attractive force of hydrogen bonds. Moreover, the two major factors that determine whether water droplets will spread across a surface are the strengths of adhesive and cohesive forces. Both adhesive and cohesive forces result from the capability of the water molecules to form a hydrogen-bonded network. Water molecules at a hydrophobic surface decreases the number of hydrogen bonds that would have pointed towards that surface, in contrast to water molecules at a hydrophilic surface, which increases the number of hydrogen bonds.

Instruments

Pre-/Post-Content Knowledge Test

The *CA-SIM* was used as a cognitive tool to gauge students' level of understanding of aqueous hydrogen bonding concepts and phenomena. The *content knowledge test* was given as both a pre- and post-intervention to students electronically as part of the CA-SIM. The pre-intervention test consisted of six multiple-choice questions of basic knowledge of hydrogen bonding (see Table I). The course professor and two graduate students with MS degrees in chemistry *validated* the pre- and post-content knowledge questions. The test served as the students' prior knowledge (PK) of this topic and was used to classify students based on their prior knowledge (High-, Mid-, or Low-PK). The post-intervention test contained the same set of questions as the pre-intervention plus six additional questions that queried their specific knowledge of the topic. These additional post-intervention items allowed students who had mastered the basic knowledge, as measured by the pre-intervention items, to be challenged on their specific knowledge of aqueous hydrogen bonding concepts. Descriptive statistics collected included the mean (*M*), standard deviation (*SD*) and post-hoc *t*-test ($\alpha = .05$), and effect size (*d* statistic) (*98*, *99*).

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Table I. Sample General Knowledge Question Item

1. Which of the following is an example of a hydrogen bond?

    (a) the attraction between the oxygen (O) and the hydrogen (H) atoms within single molecule of water
    (b) the attraction between the oxygen (O) atom of one water molecule and the oxygen (O) atom of another water molecule
    (c) the attraction between the hydrogen (H) atom of one water molecule and the hydrogen (H) atom of another water molecule
    (d) the attraction between the hydrogen (H) atom of one water molecule and the oxygen (O) atom of another water molecule

Before interacting with the CA-SIM, participants were classified into three groups based on their level of prior knowledge [similar to (*54*, *83*)] as measured by a pre-treatment score of *content knowledge* on the topic of "hydrogen bonding" (6 questions total). The High Prior Knowledge (High-PK) group was those students (49 students) who scored $\geq$ 5 correct, the Middle Prior Knowledge (Mid-PK) group (38 students) had 4 correct, and the Low Prior Knowledge (Low-PK) group (29 students) had $\leq$ 3 correct. All three PK groups interacted with the CA-SIM to explore and expand their knowledge of hydrogen-bonding concepts and phenomena in aqueous solutions.

Pre-/Post-Mental Model Assessment

The *mental model assessment* (MM form) consisted of a blank assessment form that asked students to make drawings of the hydrogen-bonding concepts and phenomena under two conditions, 25 °C and 75 °C of H_2O droplets on glass. The MM form (see an example in Figure 3) had boxes for their drawings at both the observable (MM-Obs) and molecular (MM-Mol) representation levels, and blank lines for their text to explain their drawings at both levels. This form was used with all participants to gauge their pre- and post-intervention MM's of hydrogen-bonding phenomena and concepts. To indicate experts' mental models, *content validity* was determined by administering the MM form to a professor and four doctoral students. When filling in the form, these experts express their mental models by drawing and explaining the phenomena. A rubric was created to interpret and evaluate their MM's for this topic for three relationships: (1) temperature and hydrogen bonding, (2) temperature and contact angle, and (3) hydrogen bonding and contact angle, at the observable (MM-Obs) and molecular (MM-Mol) levels (maximum and minimum scores of each level were +3 and -3, respectively).

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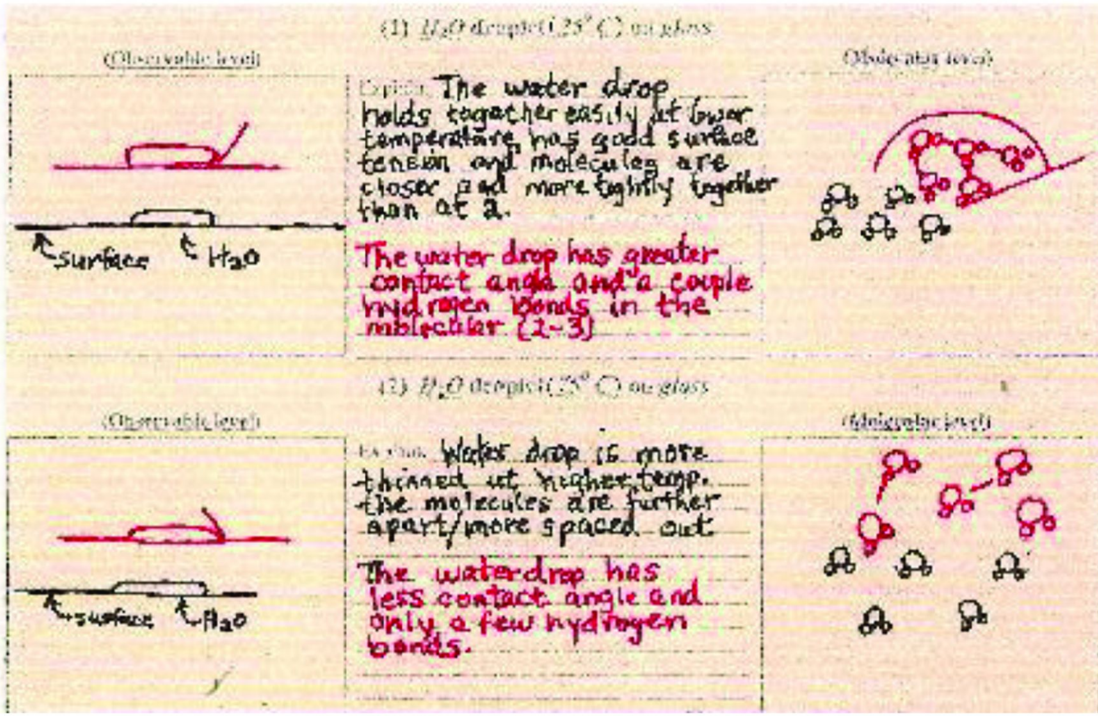

Figure 3. Example of a student's mental model (pre/post-interventions shown in black/red ink) (see color insert)

To ensure the internal consistency on the second author's mental model scoring, *inter-rater reliability* was applied to 17 randomly-selected mental models (15% of the 116). When the second author and an independent rater (a doctoral student) evaluated these mental models, they established a 73% reliability match. After discussion they reached complete agreement on the interpretation and scoring of students' mental models. For concepts at each level, (+) and (-) were used to indicate and score 'scientific conception' and 'misconception', respectively, and (0) was used to indicate and score for 'no conception'. The values for each of these dependent variables (i.e. MM-Obs and MM-Mol) are on the *interval scale*: the difference from one score to the next represents "one conception" between each integer value in the scoring rubric (e.g., -2 to -1 means moving from two misconceptions to one misconception). ANOVA with Repeated Measures (*100*) was used to measure the differences among mental model pre- and post-intervention mean scores for High-, Mid- and Low-PK groups, and the "gains" in mental model scores among these PK groups. For $p \leq .05$ measures, Cohen's *d* statistic (*98*, *101*) was used to determine the effect sizes (ES). To help the reader visualize these differences, spatial statistics (*102–105*) were applied to analyze and present central tendency and dispersion (i.e. standard deviational ellipses) of their mental model scores (Figure 4).

Experiment Data Sheet

This sheet was created so students could record the results of their investigations done with the CA-SIM. It was divided into three sections (see Figure 3 for an example). Students were prompted to record both quantitative and qualitative experimental data in order to encourage them to develop scientific conclusions for the experiments.

Perception Questionnaire

This questionnaire was adapted to evaluate perceptions of the multimedia program in Constructivist Multimedia Learning Environment Survey (CMLES) (*106*) which comprise of 15 items on 3 characteristics (i.e. dependent variables), e.g. relevance, ease of use, and challenge. The items were used to indicate level of perception of the CA-SIM upon their learning. The fifteen evaluation items were each rated on a five-point Likert scale based on how often the learning environments of the CA-SIM occurred (1 to 5 points): Almost never, Seldom, Sometimes, Often (4 points), and Always (5 points).

Interviews and Verbal Elaboration

One week after the CA-SIM, six volunteers were interviewed. In these semi-structure interviews, they were given some concrete examples of hydrogen-bonding phenomenon. They then had an opportunity to articulate their views of this phenomenon and to clarify their conceptions. In addition, the focus was on student explanations of the relationship among concepts based on their mental model in order to diagnose their "verbal elaboration", which involves "relating new information to previously learned information, creating logical relationships, drawing inferences…" ((*107*), p. 162).

Data Collection Procedures

Prior to their interaction with the CA-SIM, students performed a laboratory experiment on intermolecular forces. Then, the second author gave an orientation by explaining the purposes of the present study and the learning steps of the CA-SIM to the participants. Total time to complete the CA-SIM was approximate 40 minutes, which is described as follows:

Pre-Intervention Mental Model (5 minutes)

After a short orientation, participants completed the mental model form (see Instrumentation section). They were encouraged to use only a black ink pen to draw and explain their mental model and explanations.

Interaction with the CA-SIM (25 minutes)

After students completed the pre-intervention mental model task, they interacted with the CA-SIM individually starting with the pre-intervention of content knowledge (see Instrumentation section). All these interactions were recorded by CamStudio 2.0, which is an open source software that records all user interactions. Students also recorded experimental data on the experiment data sheet.

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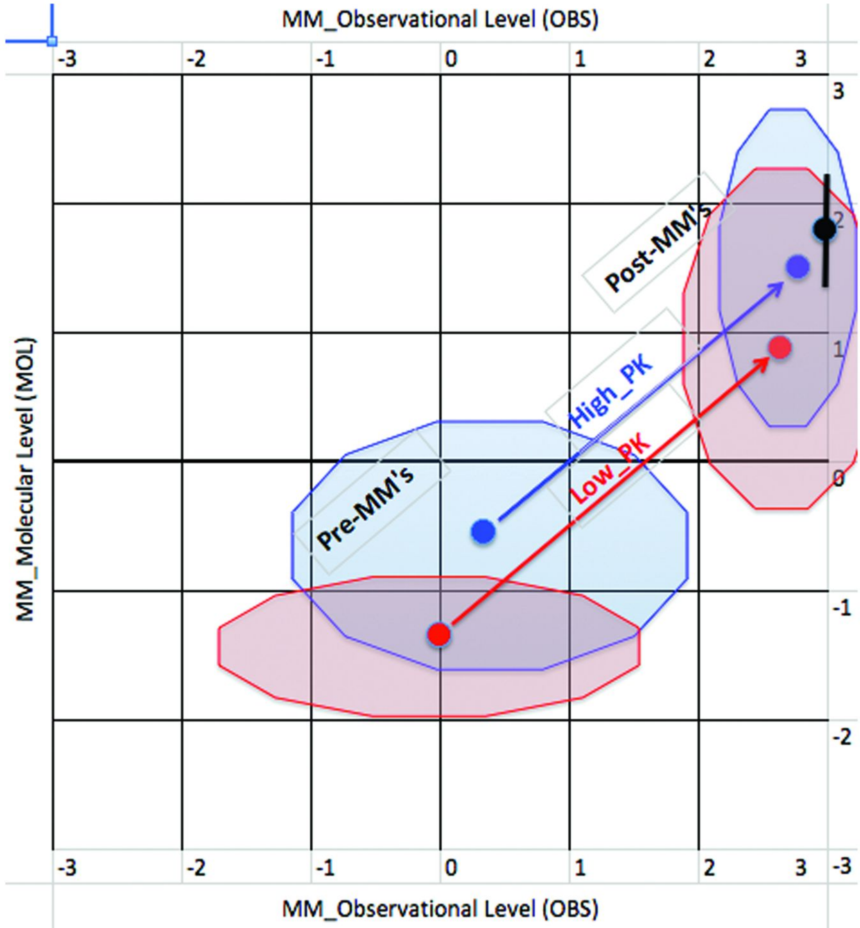

Figure 4. Mean Center (X, Y) and Standard Deviational Ellipses (SDE) for High-PK and Low-PK groups (Mid-PK omitted). Mean & SD are shown in black ink for expert conceptions.

Post-Interventions (10 minutes)

After students finished interacting with the CA-SIM, their pretest mental model form was returned to them along with *red ink pens* in order to distinguish their new markings from their original mental models, written in black ink. Thus, they could make changes in their original drawings and explanations. Next, the perception questionnaire was administered to elicit perceptions of their CA-SIM experiences.

Semi-Structured Interviews (30-45 minutes each person)

One week after students had interacted with the CA-SIM, six students volunteered to be interviewed. There were given concrete examples of hydrogen-bonding phenomena, which they discussed relative to their conceptual understanding of these phenomena. These interviews also queried their perceptions of the CA-SIM experience, and explored their mental elaboration of their mental models of the phenomena.

Limitations

Although this study of dynamic representations used real chemistry students, $N = 132$, in intact college chemistry classrooms, there were some limitations. First, among the independent variables, there was no control versus treatment group comparisons. Conversely, an ideal study should be done in artificial learning environment with a large number of students, and where each subgroup receives a different treatment based on the variables being studied (e.g., narration versus text, segmentation versus continuous animations, differential types of instructional guidance). The pre-GenK (general content knowledge) instrument should have been validated by experts and student prior to use in this study.

Results

The results for each of the three research questions were as follows:

RQ1: Do Students Gain Content Knowledge from the CA-SIM?

Table II shows the results of both the pre- and post-intervention mean scores of both general- and specific-content knowledge for students in the three PK groups (High-, Mid- & Low-PK). One-way ANOVA indicated that there was a significant difference in the post-intervention "general content knowledge" of students in the three PK groups, $F(2, 113) = 25.759$, $p < 0.001$. Specifically, the High-PK group ($M = 5.49$, $SD = 0.74$) scored significantly higher ($t = 3.567$, $p < 0.001$, Cohen's $d = 0.81$, Large Effect Size) than the Mid-PK group ($M = 4.71$, $SD = 1.18$). Also, the High-PK group scored significantly higher ($t = 8.015$, $p < 0.001$, $d = 1.93$, Very Large ES) than the Low-PK group ($M = 3.93$, SD = 0.88). The Mid-PK group out-scored the Low-PK group ($t = 3.099$, $p = 0.0014$, $d = 0.80$, Large ES). These results show that even though the Low- and Mid-PK students narrowed the gap in post-intervention content knowledge with respect to the High-PK group, this gap did not go away and the High-PK students are still consistently outscoring the other two groups. That is, these are the expected results because the same set of general content knowledge questions was used in the pre-intervention test. Conversely, on the post-intervention "specific-content knowledge" questions (i.e. relationships among hydrogen-bonding, contact angle, and temperature), there were no significant differences on scores of the three PK groups (ANOVA, $F(2, 113) = 0.531$, $p = 0.589$).

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RQ2: How Were Students' Mental Models Affected by CA-SIM?

All students' mental model (MM) drawings and explanations (e.g., see Figure 3) were interpreted and scored by the rubric score system (inter-rater reliability = 73%). On the two MM dependent variables (MM-molecular, *MM-Mol*, and MM-observational, *MM-Obs*), the descriptive statistics (*M* & *SD*) for all three PK groups (High-, Mid- & Low-PK) are shown in Table II. One-way ANOVA Repeated Measures (*SAS Statistical Program*) for the MM-Obs showed no significant differences for both pre- and post-interventions (Table III). Conversely, use of this statistic for MM-Mol produced significant differences among the three PK groups for both pre- ($F(2, 113)$ = 5.34, p = 0.0061, R^2 = 0.0864, 8.64% of variance) and post-intervention ($F(2, 113)$ = 4.71, p = 0.0109, R^2 = 0.0769, 7.69%). For the MM-Mol dependent variable, post-hoc comparisons (Table IV) were performed to identify the sources of these differences. For the pre-intervention MM-Mol's, the High-PK group (*M* = -0.69, *SD* = 0.96) outperformed both the Mid-PK group (*M* = -1.11, *SD* = 0.89; *d* = 0.446, a small effect size) and the Low-PK group (*M* = -1.31, *SD* = 0.54; *d* = 0.827, a large ES) at the α = .05 level. Note that all three PK groups had pre-MM-Mol means at the misconception end of the scale, MM-Mol < 0. ANOVA Repeated Measures program also showed that there were significant pre- to post-intervention gains for the PK groups ($F(1, 113)$ = 243.53, $p < 0.0001$). As shown in Table IV, the High-PK group's gain was from the misconceptions range (*M* = -0.69) to one in the scientific conceptions range (*M* = +1.53), which was statistically significant (Gain = +2.22, $p < 0.05$, *d* = 2.04, a very large ES). Meanwhile, the Mid-PK group showed a similar gain (Gain = +1.81, $p < .05$, *d* = 1.60, very large ES) and the Low-PK group also showed a significant gain (Gain = +2.21, $p < .05$, *d* = 1.99, very large ES). However, there were no significant differences in the gains across PK groups ($F(2, 113)$ = 1.04, p = 0.354).

In order to make these two-dimensional statistics (x = MM-Obs and y = MM-Mol) more visually comprehensible for readers (see Figure 4), we constructed a graph of observable (OBS) scientific conceptions (+x) and misconceptions (-x) on the x-axis where a student's net OBS value equals 'number of OBS conceptions' minus 'number of OBS misconceptions'. Likewise, the molecular (MM-Mol) scientific conceptions (+y) and misconceptions (-y) were used to calculate student's net MM-Mol value. Next, the Mean Center (MC) of the x-y coordinate axes (i.e. intersection of x and y means), was used to illustrate the center of the *Standard Deviational Ellipse* (SDE) for both the pre- and post-intervention MM axes. The SDE orientation of the ellipse (θ) and the two standard deviations (s_x & s_y), were used to summarize dispersion of conceptions around MC for the High- and Low-PK groups. The Mid-PK plot was omitted for clarity because there was no significant difference between Low- and Mid-PK groups. The CA-SIM learning environments positively affected students' conceptions for both High- and Low-PK groups-- as shown by the parallel lines with positive slopes from the pre-MM center of SDE to the post-MM (center of SDE). Furthermore, High-PK mental models were advanced almost to the level of experts' mental model (See Figure 4).

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Table II. Descriptive statistics, Mean & SD, for dependent variables of pre- and post-interventions.

	High PK [a] *(n = 49)*		*Mid PK (n = 38)*		*Low PK (n = 67)*	
Dependent Variables:	*Pre-*	*Post-*	*Pre-*	*Post-*	*Pre-*	*Post-*
MM-Observable	0.31 (1.53)	2.88 (0.53)	0.42 (1.57)	2.63 (1.05)	0.24 (1.60)	2.66 (0.93)
MM-Molecular	-0.69 (0.96)	1.53 (1.23)	-1.11 (0.89)	0.71 (1.39)	-1.31 (0.54)	0.90 (1.32)
Gen K [a]	5.42 (0.50) [b]	5.49 (0.74)	4.00 (0.00) [b]	4.71 (1.18)	2.65 (0.55) [b]	3.93 (0.88)
Spec K [a]	--- [c]	4.73 (1.29)	--- [c]	4.56 (1.08)	--- [c]	4.31 (1.04)

[a] PK = Prior Knowledge; GenK = General Knowledge; Spec K = Specific Knowledge [b] Student's GenK Pretest was used to define these three categories, High-, Mid-, and Low-PK. [c] No "Specific knowledge" pre-intervention was given.

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Table III. One-way ANOVA Repeated Measures for the three PK groups[a]

Dependent Variable:		*F-Value (df1, df2)*	*Significance*	*Effect size (R^{2a})*
MM-Observable	Pre-	$F(2, 226) = 0.62$	$p = 0.540$	(NS)
MM- Observable	Post-	$F(2, 226) = 1.15$	$p = 0.319$	(NS)
MM-Molecular	Pre-	$F(2, 226) = 5.34$	$p = 0.0061$	[b]
MM-Molecular	Post-	$F(2, 226) = 4.71$	$p = 0.0109$	[c]

[a] All ANOVA Repeated Measures assumptions were met for pre-/post- design (i.e. normality and homogeneity of variances). The "sphericity" assumption was not applicable because only two measures (pre-/post-) were used. [b] $R^2 = 0.0864$; R^2 corresponds to η^2, where $R^2 = (SS_{Regression})/(SS_{Total})$ Source: (*108*) [c] $R^2 = 0.0769$

Table IV. Post-hoc comparisons of MM-Molecular differences among High-, Mid- & Low-PK groups

		MM-Molecular Level		*Gain (Pre- to Post-)*
Group	*n*	*Pre-Mean [a]*	*Post-Mean [a]*	*F(1,113) = 243.53, p < 0.0001 [b]*
High-PK	49	-0.69 **A**	1.53 **A**	+2.22 **A**[c] $d = 2.04$ [L]
Mid-PK	38	-1.11 **B**	0.71 **B**	+1.81 **A**[c] $d = 1.60$ [L]
Low-PK	29	-1.31 **B**	0.90 **B**	+2.21 **A**[c] $d = 1.99$ [L]
Effect Size Comparison:			*Pre-ES [d]*	*Post-ES [d]*
High- vs Mid-PK			$d = 0.446$ [S]	$d = 0.626$ [M]
High- vs Low-PK			$d = 0.827$ [L]	$d = 0.484$ [S]
Mid- vs Low-PK			$d = 0.285$ [S]	$d = -0.142$ [NS]

[a] Means with the same letter are not significantly different at $\alpha = 0.05$ (e.g. **A = A**, **etc.**) [b] All 3 PK groups made significant gains ($p = 0.0001$) from Pre- to Post-Intervention [c] No significant differences in gains for the PK groups: $F(2, 113) = 1.04$, $p = 0.354$. [d] Cohen's post-hoc effect sizes for comparisons between PK groups, where **L** = large effect, $d \geq 0.8$; **M** = medium effect, $d \geq 0.5$; **S** = small effect, $d \geq 0.2$ (*98*, *101*).

RQ3: What Were Students' Perceptions of Their Learning Experiences from the CA-SIM?

Quantitative RQ3 Results

Overall, descriptive statistics for the *perceptions questionnaire*--the CMLES (*106*)-- indicated that the CA-SIM learning environment "often" (score of 4 on 5-point Likert scale) provided positive experiences for students. Results for the three categories of perceptions were as follows (Grand *M* & *SD*): (1) supporting

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relevant information (M = 3.94, SD = 0.54), (2) providing an easy way to learn (M = 4.32, SD = 0.65), and (3) enhancing challenges of thinking (M = 3.53, SD = 0.68). MANOVA analysis of the overall perceptions for all three PK groups showed that there were no significant differences among them ($F(3,110) = 0.48$, $p = 0.697$).

Qualitative data from the analyses of the semi-structured interviews are presented in Table V. *Qualitative RQ3 Results:* During interviews with the six student volunteers, they mentioned many positive perceptions regarding the CA-SIM. The results summarized in Table V reveals that the volunteers elaborated their conceptual understanding within the three concepts selected for analysis. These verbal elaborations were communicated in both effective (+) and ineffective (-) modes. They reflect the extent to which information that was obtained from the CA-SIM in working memory is integrated with prior knowledge structure. One of the verbal elaboration processes found in the present study is where the student added detail to the presented information and clarified an idea.

The transcriptions of two students, 'Ss A' (Low PK) and 'Ss E' (High PK), illustrate their positive perceptions that the CA-SIM helped them conceptualize their own nascent understanding by eliciting their visualizations of the phenomena.

Ss A: Before the simulation, I didn't have a conceptual understanding of this. It's like you explained this to us and sometimes it [was] hard to imagine that concept in your own life. But then I watched the simulation and begin to actually see this... the water droplets that are temperature affected and something [of the] changes in the water droplet, temperature and the contact angle. So... much more conceptual, easily understood, and I can understand pretty much better with what I saw or I see it and then I can picture it, imagine it. It's much better with conceptual [approach]. It's easier to understand the concept.

Ss E: Um... Before using the simulation, I had [a] pretty good understanding about hydrogen bonding and surface tension but after.... the simulation helped me visually understand... more clearly [than] without a diagram...

An interaction between another student, Ss C (High PK), and the Researcher (Rr, second author) gives an example of an effective mental elaboration. It indicates that the student correctly elaborated his conceptual understanding of hydrogen bonding and contact angle at both the observable and molecular levels (Table V, at MOL-3 x OBS-3).

Ss C: and then… wax is nonpolar again and it is hydrophobic. Contact angle would be very high because water would not want to be interacting with the wax surface and surface tension would be very high too.

Rr: You mean.... on the wax?

Ss C: Yes, on the wax.

Rr: Why?

Ss C: Because again.... wax is nonpolar and water is polar. So the hydrogen bonding would be very strong if it is set up at low temperature. So water would just want to be cohesive with it so and not adhesive to the wax.

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As seen from the above transcription, Student C selected words that mix everyday ideas with scientific terms (e.g. wax, nonpolar, hydrophobic, contact angle, surface tension). He also explained the properties of wax at the molecular level, e.g. nonpolar and hydrophobic, and at the relevant, observable physical properties (e.g. contact angle and surface tension). In addition, he stated the third concept, which is the relationship between hydrogen bonding and contact angle. Thus, the student associated the new material, as a description that related '*contact angle'* and *'surface tension'* of wax '*would be very high'*, with information already known, as a description *'wax is nonpolar... and it is hydrophobic'*. After the researcher questioned his reasoning, the student clarified the concepts and their relationships, *'wax is nonpolar and water is polar'* and so '*water would just want to be cohesive with it so and not adhesive to the wax'*. This transcription provides some evidence that the student used newly acquired scientific knowledge obtained from the CA-SIM and his prior knowledge to effectively elaborate his conceptual framework for this phenomenon.

Conversely, some students extended their conceptual understanding in an ineffective manner towards non-scientifically acceptable concepts. The following excerpt gives an example of a synthetic mental model (*15*) in which a student holds a correct concept but misuses one term (i.e. viscosity) in describing it. Student B (Low PK) articulated an ineffective elaborated conceptual understanding at observable level on the relationship of temperature effect on hydrogen bonding (see Table V at OBS-1 and No-MOL).

Ss B: If temperature is higher, it has higher viscosity. So higher viscosity when the temperature is high.

Rr: Why?

Ss B: Because molecules have some more energy and [are] moving faster. So they are less bonding between them because they are moving faster ... and so the contact angle would probably be very low contact angle ... I think ... um ... because more viscosity ... the responding it's gonna be having the lower contact angle ... the small contact angle. So then the low temperature, lower viscosity, and higher contact angle. So increase temperature, the viscosity is high viscosity and the contact angle is low. Here we go.

For this exchange, Student B selected words to describe his conception of the relationships among viscosity, temperature, and contact angle. His mental elaboration was based on an incorrect explanation of the relationship between different concepts (i.e. the concept of temperature and contact angle, the concept of temperature and viscosity): *'So increase temperature, the viscosity is high viscosity and the contact angle is low'*. This represents the volunteer's incorrect conceptual understanding about the observable level, where he inverted the term viscosity to mean 'ease of flow' rather than 'resistance to flow', which is the scientific definition. This verbal elaboration indicated a correct conceptual understanding about the effect of temperature on contact angle, but the wrong elaboration regarding its effect on viscosity. This ineffective elaboration occured because the student used a prior misconception of '*If temperature is higher, it*

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is higher viscosity' to connect new-coming information from CA-SIM to his existing knowledge.

Overall, these empirical results on student's mental elaborations, as seen in Table V, strongly reveals that students could form meaningful scientific understanding by integrating scientific knowledge obtained from the CA-SIM learning environments into their existing knowledge framework. It also reveals how misconceptions in existing knowledge can get intermingled with incoming information to form 'synthetic conceptions' (*15*, *109*) that are discussed in the following section.

Table V. Distribution for the 6 Interviewees (A - F) of Students' Conceptions and Mental Elaborations for Hydrogen-bonding Phenomena at the Observable (OBS columns) and Molecular (MOL rows) Levels.

	No OBS Conceptions	*OBS-1: Temp ~ H-bonding*	*OBS-2: Temp ~ Contract Angle*	*OBS-3: H-bonding ~ Contact Angle*
MOL-3: H-bonding ~ Contact Angle	**+C, +F** **-F**	**+F**		**+2B, +2C, +D, +E, +3F**
MOL-2: Temp ~ Contact Angle	**+E**	**+E**		
MOL-1: Temp ~ H-bonding	**+F**	**+3C, +4D, +E, +F** **-A, -C**		
No MOL Conceptions		**+2A, +3B, +D, +F** **-2B**	**+A, +E**	

NOTE: For both the OBS columns and MOL rows: Letters (A, B, …) refer to students who were interviewed. Low-PK Students were **A** and **B,** and High-PK students were **C** through **F**. Misconceptions are negative (e.g. **–A**) and scientific conceptions are positive (e.g. **+A)**. Numbers in front of letters refer to the number of times the student discussed that particular concept (e.g. +2B means two constructive comments from Student 'B').

Discussion

Impact of Prior Knowledge on Content Knowledge

Results for Research Question 1 (RQ1) showed the effect of the CA-SIM on post-intervention *content knowledge* of hydrogen-bonding phenomena. That is, the High-PK students scored significantly higher than Mid-PK, who, in-turn scored higher than the Low-PK students. In other words, the Low- and Mid-PK groups did not learn enough content knowledge from the simulation to reach the level of those who initially possessed a relatively high level of content knowledge about hydrogen-bonding concepts. Their lack of gain in content knowledge may be due to their inability to fully verbalize their multimedia experiences, which were predominantly visual representations with verbal instructional support. This lack of transfer among different representations of a phenomenon may mean that the Low- and Mid-PK students were not able to fully make a meaningful transition from their *experiences* with both the phenomenon in the real laboratory experiment and the multimedia representations of CA-SIM towards the theoretical *model* (*73*). Experiences and model-construction are two distinct types of knowledge (*73*), which often take years to integrate as illustrated by conceptual development in children (*110*) and the development of a particular expertise (*111*).

Impact of Prior Knowledge on Development of Mental Models

Results for RQ2 showed that the CA-SIM helped all students improve their mental models at both the observable level (macroscopic, MM-Obs) and molecular level (submicroscopic, MM-Mol). At the observable level, High-, Mid- and Low-PK students used the CA-SIM to develop their MM-Obs mental models at the same rate (i.e. no significant *F*-values for pre- or post-intervention MM-Obs scores, Table III). Conversely, at the molecular level, the CA-SIM could not help the Low- and Mid-PK students close the gap between their MM-Mol models and those of the High-PK students (i.e. see Table III). This empirical evidence suggests that the CA-SIM helped all three PK groups to improve the accuracy of their constructed mental models (Figure 4) by reducing their misconceptions while allowing them to acquire more scientifically acceptable mental models.

The combined model (see Figure 1) is based on Mayer's cognitive theory of multimedia learning (*76*) and Schnotz and Bannert's integrated model of text and picture comprehension (*74*). Mayer's model clearly shows that students' *prior knowledge* plays an essential role in their ability to form an integrated mental model from their complementary verbal and pictorial models. Meanwhile, Schnotz and Bannert's model (*74*) emphasizes that there are two distinctive types of representations—i.e. *descriptive representations* resulting from symbol processing (i.e. word semantics and mathematical equations) while *depictive representations* result from analogical structure mapping. They state that task-appropriate pictures are likely to support the mental-model construction process, while task-inappropriate pictures may interfere with this process (*74*). In this study, all students, regardless of their level of prior knowledge, greatly enhanced their mental models of the hydrogen-bonding concepts and phenomena (see Figure 4). Thus, the level of instructional guidance (see *Instructional*

Materials section) in the CA-SIM was appropriate due to the fact that previous studies have shown that low PK students vitally need instructional support. They used this guidance to reduce their level of cognitive load to a manageable level while learning within a context that allows them to integrate their limited knowledge with the new information provided in CA-SIM (*68*, *77*, *89*). Evidence for this support was that the rate of conceptual development (i.e. pre- to post-) towards coherent mental models for the Low- and Mid-PK students *paralleled* that of the High-PK students (Figure 4). Previous studies have shown that when an animation provides support for step-by-step integration of information, then the performances of all students can benefit, and the gap between the various PK levels remains constant (*54*, *77*). Conversely, when multimedia does not include instructional help, the gap between the high-PK and mid-/low-PK students widens [Figure 2 in (*54*)].

A previous study by Corradi et al. (*83*) found that low and high PK students responded differently to different types of instructional guidance. That is, low PK students, but not high PK students, benefitted from prompting, where a guiding question directed their attention away from text and towards more symbolic representations. Thus, prompting in the form of *cues* (i.e. multimedia features that guide students to relevant information) helped low PK students (*86*, *112*). In this study, cues were an integral part of the CA-SIM instructional design (see *Instructional Methods* section). Corradi et al. found that high-PK students were adversely affected by this same prompting help. These researchers reasoned that high-PK students would have been better supported by "drawing representations… in supporting [their] metacognitive understanding (p 793)", which would have allowed them to create links among all three chemical representations—submicroscopic (molecular), symbolic (chemical formulas and equations; mathematical equations), and textual (words). In the present study, all students were encouraged to *draw* their visual representations and *explain* their textual representations to illustrate their mental models of the hydrogen-bonding concepts and phenomena (e.g., see Figure 3). While the animated CA-SIM may have benefitted the High-PK students, drawing and explaining representations from an animation helps all students understand the chemical processes and concepts (*51*, *65*) because it is no more demanding than reading/ viewing these representations (*72*). Furthermore, it can lead to a deeper conceptual understanding (*65*, *66*).

When the participants learned hydrogen-bonding phenomena and concepts from the CA-SIM (see Figure 4), the mental models of all three PK groups (Low-, Mid- & High-PK) were considerably enhanced at both the observational (MM-Obs) and molecular (MM-Mol) levels. This increased student accuracy approached scientific acceptable mental models as indicated by the proximity to experts' mental models (Figure 4). Thus, it could be argued that the CA-SIM significantly influenced a transformation in students' mental models from simple to more complex mental models via two related learning pathways. First, it alleviated their misconceptions (*64*) as shown by the shift in both MM-Obs and MM-Mol away from the "net misconceptions" (i.e. negative integers in Figure 4). Second, it supported their acquisition of scientifically correct conceptions for all three hydrogen-bonding conceptions as indicated by their "net positive" post-intervention conceptions, which were embedded within their mental model networks (*15*, *109*). Rhodes (*113*) pointed out that simulations and modeling could help students understand complexity of natural phenomena. Thus, we believe that the students had opportunities to change and restructure their own conceptions and then transform and remodel the phenomena by incorporating it into their own new mental models.

Furthermore, the results shown in Figure 4 also show the CA-SIM's impact in helping most students develop good mental models on the observable level of the phenomenon; however, no student had a fully developed mental model at the molecular level after experiencing the CA-SIM learning activity. This evidence could be argued that the CA-SIM has a potential limitation for helping in the mental model construction process. Haag and Kaupenjohann (*114*) mentioned that simulations have limited predictive capacity, where it is difficult to validate this mental process. Therefore, students could construct differences in their content knowledge, and this situation could result in conceptual dispersion (*115*). Conversely, the CA-SIM exerted an impact on their mental models with varying degrees of success in that it essentially united improvement on student's OBS mental models but did not result in uniform improvement of their MOL mental models. Haag and Kaupenjohann (*114*) also reported that dynamic simulations offer a remarkable potential for consensus mental model building.

Overall, these results are consistent with the research findings that students performed better when learning from computer simulations (*33*, *40–44*, *64*, *116*). Additionally, Tasker and Dalton (*64*) reported that computer visualization enhanced students' numbers of scientifically acceptable conceptions, allowed them to develop more vivid mental imagery, and transferred their ideas to new situations. Frederiksen, White, and Gutwill (*116*) also reported the benefit of computer simulations in that the dynamic nature helped students create a clearer appreciation of the conceptual linkage between scientific knowledge objects and an aggregated model, which represents physical phenomena at different levels of abstraction. However, in this empirical study, it could be argued that students' prior knowledge was also needed to develop a better understanding of the phenomena and to develop mental models that approached the mental models of experts (see Figure 4). This argument is consistent with claims that students' level of pre-knowledge affects what they learn from simulations (*41*, *117*).

Roles of Perceptions in Supporting Deep Understanding

Quantitative results for RQ3 indicated that almost all of the students had favorable perceptions toward the CA-SIM learning environment. Overall, they had positive perceptions for each characteristic of the CA-SIM; however, there were no significant differences for the Low-, Mid- & High-PK groups. Most of the students perceived that the CA-SIM presented authentic information, which was representative of real-life situations, represented the data in a variety of ways, and challenged and stimulated them to do more thinking.

The qualitative results for RQ3 from the interviews with selected students revealed that the CA-SIM stimulated students' mental elaboration processes, e.g. adding detail to the information, and clarifying their associations between the new material and the information they knew from past experiences. These volunteers also explained the relationships between different concepts based on their new conceptual learning, which was constructed based on their interactions with the CA-SIM. Such mental elaborations make the new conceptual understanding more meaningful. This cognitive process of mental elaboration could allow students to develop meaningful conceptual learning, but only if their elaborations were compatible with their prior knowledge (*118*). Elaborations can help an individual develop a richer and deeper understanding, while constructing complex mental models (*119*). Conversely, results of this study showed that students in all three PK groups (Low-, Mid- & High-PK) had opportunities to build both effective and ineffective mental elaborations. That is, when weaker formal pre-knowledge is intertwined with deeply rooted misconceptions, students tend to form ineffective mental elaborations. This process can obstruct their development of meaningful conceptual understanding (*118*). Thus, low initial chemistry knowledge (low PK) means they are more likely to integrate their misconceptions into their mental elaboration processes. Consequently, the elaborated information they develop often results in non-beneficial learning (*118*).

Conclusions and Implications

Previous research has investigated the impacts of computer simulations on students' learning of scientific concepts and on students' mental models of chemical bonding and processes (*6*, *73*, *78–80*, *120*). However, very little research has examined students' conceptions of hydrogen bonding phenomena, while none have studied the effectiveness of computer simulations in enhancing students' conceptions of aqueous hydrogen-bonding and contact angle in water droplets. The overall results of this study suggest that the CA-SIM learning environment provided opportunities for students to explore the phenomena and to provoke new scientific thinking about these phenomena. Because of these features (see *Instructional Materials* section), the CA-SIM learning environment has the capability to help students develop domain content knowledge while restructuring their misconceptions into accepted scientific conceptions.

When these results (i.e. RQ1, RQ2 & RQ3) are combined, the evidence suggests that the design of CA-SIM was successful at reducing working memory load from visual and verbal representations, while facilitating student integration between the new and their existing scientific knowledge. Thus, most students tended to have positive perceptions that may have helped encourage development of more scientifically correct mental models. These perceptions may have been associated with a deeper conceptual understanding that resulted from their interaction with the CA-SIM. Likewise, Wekesa, Kiboss, and Ndirangu (*121*) reported that computer-based simulations positively affected the development of students' understanding and perceptions of their learning experiences. Also, Supasorn, Suits, Jones, and Vibuljan (*122*) reported that students perceived a computer simulation as being an effective tool to help them visualize scientific concepts at both the macroscopic and microscopic levels.

Overall, these findings on student use of the CA-SIM provide insight about the potential of animations and simulations to support students' construction of

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meaningful understanding of chemical phenomenon and its representations. The CA-SIM learning environment also used an everyday phenomenon (i.e. water droplet on a solid surface) to enhance and support their conceptualizations of hydrogen bonding and related concepts at both the observable and unobservable levels. Animations and simulations could thus help students eliminate their misconceptions (i.e. alternative conceptions) while developing their scientific knowledge of real life phenomena.

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Chapter 11

Making the Unseen Seen: Integrating 3D Molecular Visualizations in Elementary, High School, and Higher Education

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This chapter describes three studies that attempted to change the predominant traditional lecture-based instruction by integrating 3D visualizations into chemistry courses. The three studies had one similar objective: to examine the effect of 3D web-based molecular visualizations on students' learning outcomes, centering on five cognitive abilities. The studies were conducted among elementary, high school, and university students. Data were collected by applying quantitative methods within a pre- and post-experimental design. The findings in all three studies suggested that in order to enhance the construction of scientifically correct mental models, students should be engaged in the construction and manipulation of 3D visualizations. Passive observations of 2D molecular drawings in textbooks or even teachers' demonstrations of 3D molecular visualizations are not sufficient for enhancing higher levels of cognitive abilities. Among the many advantages of using advanced technologies in chemical education, web-based visualizations are significantly important for helping students to "see the unseen", thus improving their chemical understanding.

Introduction

In the past two decades, an increasing number of educators are abandoning teacher-centered, lecture-based modes of instruction, moving towards more learner-centered models (*1*). This shift is in response to the ongoing criticism about

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the domination of lecture-based teaching that induces shallow understandings of the learning material (*2*, *3*). Motivated by a desire to change the predominant lecture-based teaching mode, and building on the constructivism learning theory, educators encourage the development of active learning environments. In active learning environments, students are involved in more than listening passively. Emphasis is placed less on transmitting information and more on developing students' cognitive and operative skills (*4*). Active learning environments enable learners to create their own mental framework and formulate their own conceptual models (*5*). In chemical education, the use of 3D molecular visualizations can promote active learning by encouraging students to solve problems, provide explanations, manipulate 3D visualizations, and construct computerized models. Integrating active learning strategies as part of the formal learning sessions can advance students' learning as well as address the need for a pedagogical change (*6*).

This chapter includes a literature review on internal and external visualizations and the use of three dimensional (3D) visualization in chemical education. It provides an overall view of three chemistry courses in elementary, high school, and higher education. It then describes three related studies that examined the integration of web-based 3D molecular visualizations and their effect of students' learning outcomes. Finally, the summary and discussion section provides some new insights regarding the use of visualizations for chemical education.

Internal and External Visualizations and Chemical Education

Visualization is conceptualized as a basic form of cognition and it plays a central role in our imagery, abstraction, and creativity abilities. Visualization exists internally, as a mental image in our mind. But it also exists externally, as a 3D physical model, a 2D drawing on paper, or an image on a computer screen. Internal and external visualizations are mutually reliant, depending on the level of abstraction and the individual's imagery/spatial ability. Those who have low imagery ability use external visualizations in order to better understand complex and abstract ideas. Those who have high imagery ability do not need external visualizations for understanding complex phenomena; however, they can present visual models in order to convey their knowledge and ideas to others (*7*). External visualizations may augment internal visualizations by providing additional information or insights. It can present a more complex process than can be internally visualized within a persons' limited capacity of visual-spatial working memory (*7*).

In recent years, advances in technology have improved the ability to create external visualizations. Developments in multimedia capabilities (graphics, audio, and video) made it possible to produce powerful visualizations of abstract scientific phenomena and processes (*8–10*). According to Mayer's dual coding theory on learning and multimedia (*11*), there are two separate channels for processing information: visual-pictorial and auditory-verbal, both mutually important for enhancing meaningful and deep learning. Indeed, studies indicated that by providing well-designed external visualizations, such as colorful, 3D molecular representations, students can construct internal visual representations and thus enhance their learning outcomes (*8*, *12*). Williamson and Abraham (*12*) found that students who used external visualizations in the form of molecular animations, improved their conceptual understanding of the particulate nature of chemical reactions, compared to those who studied chemistry in a traditional way. Similarly, Barak and Dori (*8*) found that the use of external visualizations enhanced students' conceptual understanding and modeling skills.

External visualizations such as physical or computerized models, animations, and/or interactive simulations can be integrated into the teaching and learning processes for describing, explaining, and discussing scientific phenomena. They can illustrate complex phenomena on a macroscopic level or by "zooming in" into the microscopic level. In the chemistry discipline, 3D computerized representations are well-integrated into research and teaching. In general, there are three types of computerized representations of molecules: those that present animations of chemical processes and/or reaction pathways; those that allow the manipulation of molecular models - rotating, changing representation modes, measuring lengths of bonds, etc.; and those that facilitate the modification of molecular models and the construction of new models. These visualization tools transfer abstract ideas into concrete ones, thus help teachers explain complex phenomena and help students understand chemical concepts and processes (*8*, *13*).

The use of computerized molecular representations has been studied since the 1990's by many chemical education researchers. In 1995, Williamson and Abraham (*12*) reported that animations enhance students' understanding of chemical concepts and promote their ability to construct dynamic mental models of chemical processes. Lipkowitz and colleagues (*14*) used visual representations for teaching the topic of mineralogy and as a bridge between the disciplines of geology and chemistry. Kantardjieff and colleagues (*15*) introduced 3D visualizations while using Silicon Graphics workstations, engaging students in exploration activities. Later on, at the beginning of the new millennium, Sanger and colleagues (*16*) used computer visualizations to help students understand chemical processes. They found that students who used computer visualizations were less likely to quote memorized mathematical relationships and more likely to understand abstract concepts and phenomena. Fleming and his colleagues (*17*) developed an animation package that animated reaction pathways. They presented a new teaching approach for constructing an understanding of molecular orbital interactions. In 2001, Donovan and Nakhleh (*18*) indicated that the web-based representations used in their general chemistry course were instrumental in visualizing and understanding chemistry. These results were in line with the findings of Dori and colleagues (*19*), indicating that the use of web-based molecular 3D visualizations positively effected students' achievements, provided the students are actively engaged in constructing the computerized models. In summary, studies indicated that 3D visualizations enhances students' spatial abilities (*13*), learning achievements (*18*, *19*), conceptual understanding (*8*, *12*), and motivation to learn science (*20*).

Since chemistry learning involves the understanding of abstract phenomena, 3D visualizations are applied in order to disclose the "unseen". Indeed, visualizations enable the creation of mental representations of complex concepts and it can substitute for cognitive processes, such as: abstraction, imagination, or creativity, that some students lack. However, ill-designed and oversimplified visualizations may cause misunderstandings among students. In addition, they may harm the learning process by preventing the use of ones' own imagination, and thus, hinder the creation of mental models (*21*). If the visualizations are ill-designed and too much or too little information is displayed, they may prevent learners from performing effortful cognitive processes required for a deeper understanding (*21*). Choosing well-designed 3D visualizations and incorporating them as an integral part of the learning process is significant for effective and meaningful learning. Following this line of thought, this chapter describes three studies that integrated web-based 3D molecular visualizations into chemistry learning while examining students' learning outcomes.

Three Studies: An Overall View

This chapter describes three studies with one similar objective: to examine the effect of web-based 3D molecular visualizations on students' learning outcomes. Each study was conducted among a different research population: elementary, high school, and university students. The first study describes the integration of 3D animations into elementary school science curriculum, examining students' chemical understanding, explanation skills, and motivation to learn science. The second study describes the integration of 3D molecular visualizations of proteins' structure and function into the curriculum of high school chemistry courses. It examined whether, and to what extent, learning via visualizations of biomolecules effect students' chemical understanding. The third study describes the use of visualization software for the construction of dynamic molecular models. This study examined university students' conceptual understanding and their ability to transfer across the four levels of chemical understanding: macroscopic, microscopic, symbol, and process (*19*). In all three studies, the experimental groups used 3D visualizations as part of their learning process. They were engaged in assignments that could only be answered after they truly understood the scientific concepts and phenomena presented in the 3D molecular visualizations. Conversely, the control groups were taught in a traditional way, by using textbooks with static 2D pictures of molecular models.

As described above, the three studies were similar; but, there were two main differences: the participants' age (elementary, high school, and university) and the applied visualization software. Based on the constructivism theory, all experimental students were actively engaged in the learning process; however, their ability to manipulate the computerized molecular models depended on the software's capabilities. The elementary students were mostly engaged in observing funny and entertaining animated movies created by BrainPop (http://www.brainpop.com). Most animated movies included a "zoom in" effect (from macro to micro), allowing the young students to "see" the structure and behavior of molecules in various situations. The high school students used the Side-by-Side Images

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of Amino Acids' website, developed by Carnegie Mellon University (https://www.bio.cmu.edu/courses/03231/BBlocks/AAVFrameset.htm), allowing them to compare 3D structures of amino acids and peptides. They rotated the molecular models and changed their representation modes from ball and stick to space-fill or sticks. They measured the length of the bonds (in Å units) and indicated the polarity of each side chain. The university students used MDL ISIS Draw (http://mdl-isis-draw.software.informer.com) for drawing structural formulas, and ViewerLite 5.0 (http://viewerlite.software.informer.com/5.0) for viewing the 3D computerized models. They did all the activities that the high school students did, with the addition of constructing the molecular models on their own.

In all three studies, data were collected by applying the quantitative method, within a pre- and post-experimental design (*22*), using the general linear model (GLM) for statistical analysis. Analysis of Covariance (ANCOVA) was used to compare post-questionnaire scores while holding the pre-questionnaire scores "constant" for a validated comparison.

Study 1: Integrating Animations into Elementary School Science Education

The first study was conducted in the context of reforms in elementary school science education in Israel. The study examined a program that integrated web-based animated movies, created by BrainPop (http://www.brainpop.com), into the curriculum of grade four and five students. Each animated movie is 3-to-5 minutes long, providing explanations about scientific concepts in an entertaining and dynamic way. Each movie includes animated characters who lead students through educational activities, while providing curriculum-based contents that are aligned with the national science education standards. The teachers' section contains lesson plans, laboratory experiments, and ideas for using BrainPop animations in the classroom.

Study 1 Research Questions and Participants

In order to examine the effect of web-based 3D molecular visualizations on elementary school students' learning outcomes, the following research question was raised: Whether and to what extent the use of visualizations effect students': conceptual understanding, explanation skills, and motivation to learn science?

The research participants were divided into two groups: experimental and control, according to the preferences of the science teachers. The experimental group included 926 students from five elementary schools, composed of 435 fourth graders and 491 fifth graders. The control group included 409 students from two elementary schools, composed of 206 fourth graders and 203 fifth graders. Among the 14 science teachers that participated in the study, nine taught the experimental students and five taught the control students. Among them, there were two teachers who taught in both experimental and control schools. In such large scale studies, the distribution of good and poor teachers among both research groups is similar.

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The experimental schools integrated the animated movies at least once a week, about one animation for each topic. The teachers demonstrated the animated movies to their students in the classroom and encouraged them to work on their own or in pairs in computer clusters. The students watched the animations while answering questions or carrying out learning assignments. The animations comprise of animated characters who lead the students through educational activities, including 3D visualizations of particle movement and structure. The topics in "Matter and Chemistry" include: atomic model, body chemistry, chemical bonds, state of matter, compounds and mixtures, and more. Differing from the experimental group students, the control group students studied the science courses in a traditional way – using textbooks with still-pictures and exercise sheets.

Gender distribution was close to even, almost 13% declared that they participate in extracurricular activities in science education, and only about 10% declared that their parents' occupation relates to science (medical doctors, scientists, engineers etc.). Pearson Chi-Square test indicated no statistically significant differences between the research groups in respect to gender distribution, class distribution, parents' occupation, and extracurricular activities.

Study 1 Pre- and Post-Questionnaires

The pre- and post-questionnaires administered in this study consisted of four parts. The first part indicated the students' demographic details, such as: class, gender, parents' occupation, and extracurricular activities. The second part examined students' conceptual understanding. It included eight multiple-choice questions, based on national science standards and topics, such as: natural materials and substances, energy preservation, living organism, etc. The third part examined students' explanation skills. It included four true/false questions with a requirement to write an explanation for each choice. The fourth part examined students' motivation to learn science. It included 20 items on a 1-to-5 Likert-type scale, divided into four categories: Self-efficacy, Interest and enjoyment, Connection to daily living, and Importance to the student. This part was adapted from Glynn and Koballa (*23*), modified to fit elementary school students, and has been published in Barak, Ashkar, and Dori (*20*).

The pre- and post-questionnaires were similar in their construct, but with different contents for the 4th and 5th grade students, according to the themes taught in each cohort. Each of the 4th and 5th grade questionnaires had two versions with the same questions displayed in a different order. The students who received version A as their pre-questionnaire, were given version B as their post-questionnaire, and vice versa. The questionnaires were validated by four experts in science education and three elementary school teachers, reaching 100% consent. The reliability, determined by internal consistency, Alpha Cronbach was 0.88 for the motivation section. The questionnaires were administered to the students at the beginning and the end of the academic year.

Study 1 Findings

The findings section includes two parts. The first part presents students' understanding of scientific concepts and their explanation ability. The second part presents students' motivation to learn science.

Students' Understanding of Scientific Concepts and Their Explanation Ability

ANCOVA test indicated that the difference in students' gained conceptual understanding can only be explained by their participation in the BrainPop animated movies program ($F_{(1,\ 1332)}$=127.50, $p<0.001$), and not by gender differences, parents' occupation, or participation in extracurricular activities. In other words, students who experienced the use of animated movies as part of their learning process improved their understanding of science concepts and phenomenon, in comparison to students who used only textbooks and 2D still-pictures.

The students' explanation to the true/false questions were analyzed and categorized into four explanation levels:

1. Correct explanation – providing scientific data and a solid rational.
2. Partial explanation – providing incomplete or partial scientific data.
3. Incorrect explanation – providing an incorrect answer or irrelevant details.
4. Missing explanation – providing no explanation at all.

For instance, the students were asked to indicate whether the metal "Gold" should be used for producing electrical wires and explain their answer. Examples of students' responses divided by explanation levels are presented in Table I.

Comparing 4th grade students' levels of explanations, ANCOVA test showed that the experimental group students indicated statistically significant higher percentages of correct explanations compared to the control group ($F_{(1,\ 623)}$=7.10 $p<0.05$). Eta Squared analysis indicated that 22.0% of the growth in students' explanation skills can be accounted for the use of animation. No statistically significant difference was found between the research groups in percentage of partial, incorrect, or missing explanations.

The comparison of 5th grade students' levels of explanations showed that the experimental group students had a higher percentage of correct explanations compared to the control group. However, ANCOVA test indicated no statistically significant difference between the research groups in percentage of correct, partial, incorrect, or missing explanations among grade five students. This can be due to the relatively simple question that was presented to grade five students. This question was easy for them to answer and explain, and did not require much imagery or abstraction skills.

Table I. Examples of students' answers divided by explanation levels

Students' answers	*Score*	*Explanation*
Although it has relative high conductivity, this metal is not good for producing electrical wires since it is too expensive. *Gold is a good conductor, but it is also very expensive. Electrical wires that will be made of gold will likely be stolen and this will cause many electrical breaks.*	3	Correct
This metal is a good conductor but not good for producing electrical wires since they should be made of copper. *Gold has good conductivity, but it should not be used for wires but for preparing jewelry.*	2	Partial
Gold is good for producing electrical wires since it is made from metal. *It is a good conductor and it should be used as electrical cables.*	0	Incorrect

Students' Motivation To Learn Science

The pre- and post-questionnaires net-gains for students' motivation to learn science were calculated for each of the four categories, divided by research groups. Figure 1 shows that in all of the categories, the experimental group students indicated an increase in their motivation to learn science as result of learning with animations, compared to the control group students.

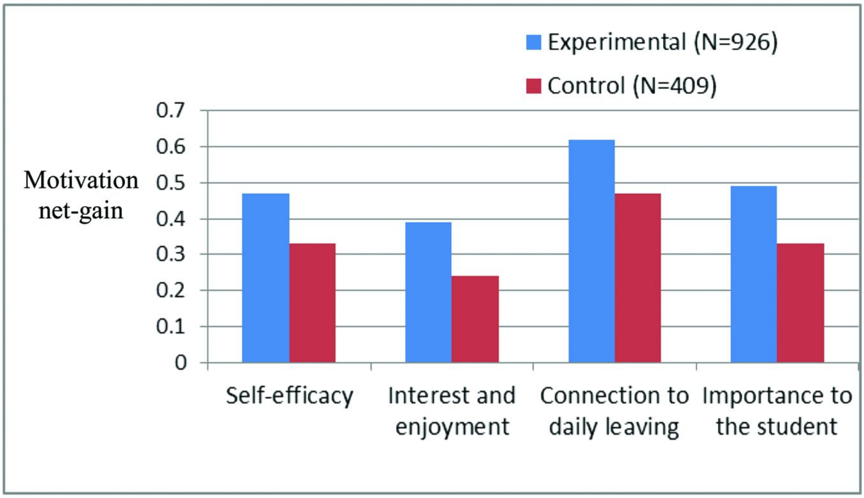

Figure 1. Students' motivation net-gain by categories and research groups (see color insert)

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While applying ANCOVA test, findings indicated that the experimental group students asserted statistically significant higher motivation, compared to the control group students ($F_{(1, 1332)}=53.48$, $p<0.001$). This result suggests that the use of animated movies enhances students' motivation to learn science, rather than just using textbooks and still-pictures. Pearson correlations between students' increase (net-gain) in motivation to learn science and their learning outcomes indicated positive correlations for both research groups: experimental and control ($r=0.21$, $p<0.001$; $r=0.13$, $p<0.05$, respectively). This result suggests that throughout the academic year all students developed scientific understanding, parallel to developing positive motivation toward science learning. However, the correlation between the two variables (motivation and learning outcomes) among the experimental group students was almost twice as high compared to the control group students.

The results of Study 1 are further elaborated by Barak and Dori (*9*) and by Barak, Ashkar and Dori (*20*). The positive findings can be explained by the fact that while exploring animated movies, the students apply two cognitive channels: visual-pictorial and auditory-verbal. Both channels are simultaneously applied enabling the construction of mental models that are close to those of expert scientist.

Study 2: Integrating Molecular Visualizations into High-School Chemical Education

The second study was conducted in the context of high school chemistry education reforms in Israel. The study examined a new biochemistry learning unit that was developed to promote in-depth understanding of 3D structure and function of biomolecules for grade 12 students. The learning unit encouraged active exploration of web-based visualizations, developed by various universities in the US. The students that studied the new biochemistry unit experienced the use of "Side-by-Side Images of Amino Acids" (https://www.bio.cmu.edu/courses/03231/BBlocks/AAVFrameset.htm) developed by Carnegie Mellon University.

Study 2 Research Questions and Participants

In order to examine the effect of web-based 3D molecular visualizations on high school students' learning outcomes, the following research questions were raised: Whether and to what extent the use of visualizations effect students':

1. Knowledge, comprehension, and application of proteins' structure and function?
2. Ability to transfer across molecular representation modes and chemical understanding levels?

The research included a representative sample of 175 grade 12 students, divided into three research groups: two experimental and one control.

a) Experimental I - Students who studied the new biochemistry learning unit while exploring dynamic 3D visualizations on their own (N=51). The students were actively engaged in manipulating molecular models, rotating them, and calculating angles and distances between atoms. They were applying kinesthetic-hands-on learning.
b) Experimental II - Students who studied the new biochemistry learning unit while the teachers presented the dynamic 3D visualizations on a large screen in the classroom (N=63).
c) Control - Students who studied according to the traditional curriculum while viewing static 2D illustrations of molecules in textbooks (N=61).

Chi-square analysis indicated no statistical significant difference between research groups by gender and demographic background. Students from all three research groups studied the topic of *Proteins' structure and function* for the same amount of time - 20 hours, in a period of five weeks.

Study 2 Pre- and Post-Questionnaires

The pre- and post-questionnaires administered in this study were based on similar questionnaires developed by (*8*), adapted to the contents of proteins' structure and function. The pre-questionnaire was designed to examine students' prior knowledge in chemistry and the post-questionnaire investigated their gained knowledge. Both questionnaires consisted of five assignments. Three assignments were identical in the pre- and post-questionnaires; designed to indicate students' knowledge, comprehension, and application of proteins' structure and function. The fourth assignment was designed to indicate students' ability to transfer across the three modes of molecular representation: three dimensional (3D), two-dimensional (2D), and textual. The pre-questionnaire referred to simple molecules: ammonia, acetic acid, and water. The post-questionnaire included amino acids: alanine, cysteine, and aspartic acid. The fifth and last assignment was designed to indicate students' ability to transfer across the four levels of chemical understanding: macroscopic, microscopic, symbol, and process (*19*, *24*). The pre-questionnaire included methanol, glycine, and hydrogen sulfide. The post-questionnaire included amino acids: valine, serine, and glycine.

The questionnaires' reliability was established by Barak and Dori (*8*). Content validity was established in this study by three chemical education experts. The experts indicated full agreement as to the extent to which the questionnaires truly measure students' knowledge, comprehension, and application of proteins' structure and function.

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Study 2 Findings

The findings section includes two parts. The first part presents students' knowledge, comprehension, and application of protein structure and function. The second part presents students' ability to transfer across the three modes of molecular representations and across the four levels of chemical understanding.

Students' Knowledge, Comprehension, and Application of Proteins' Structure and Function

Students' knowledge, comprehension, and application of protein structure and function were examined by three assignments. Following Bloom's taxonomy (*25*) the first assignment was indicated as a *knowledge* question, requiring a solution for a chemical process. The second assignment was indicated as a *comprehension* question, requiring the description of amino acids' properties and structure. The third question was indicated as an *application* question, requiring the establishment of connections between knowledge on proteins, and their structure and functionality in the human body.

While examining students' performance on the first assignment, an ANCOVA test indicated statistically significant differences between the three research groups ($F_{(2,\ 170)}=3.392$, $p<0.05$) in their *knowledge* of chemical concepts. Post Hoc Sidak test showed that the post-questionnaire mean score of the control group was statistically significant lower than that of the two experimental groups.

While examining students' performance on the second assignment, ANCOVA test indicated statistically significant differences between the three research groups ($F_{(2,\ 170)}=10.40$, $p<0.01$) in their *comprehension* of chemical concepts. Post Hoc Sidak test showed that the post-questionnaire mean score of the students who explored and manipulated the molecular visualizations, was statistically significant higher than that of the other two research groups. Examples of the students' responses and their assigned scores (out of 10 points) by levels of chemical understanding are presented in Table II.

While examining students' performance on the third assignment, an ANCOVA test indicated statistically significant differences between the three research groups ($F_{(2,\ 170)}=4.31$, $p<0.05$) in their *application* ability. Similar to the previous result, Post Hoc Sidak test showed that the post-questionnaire mean score of "Experimental I" group was higher than that of the other two research groups. This result suggests that learning proteins via exploration of web-based models and visualizations improves students' application ability, which is the third cognitive level in Bloom's taxonomy (*25*).

Table II. Examples of students' responses to the assignment that examined their chemical understanding

Students' responses	*Score*	*Levels of chemical understanding*
Amino acids can react both as acids and basis. They have an amino group (-NH_2) which attracts a proton (H^+) due to a pair of non-bounding electrons on the nitrogen atom, thus acting as basis. They also have a carboxylic group (-COOH) which releases a proton, thus acting as acids.	10	Macroscopic, Microscopic, Symbol, and Process
Amino acids consists of both an amino group (-NH_2) and a carboxylic group (-COOH).	5	Microscopic and Symbol
Amino acids consist of a hydrophilic group and a hydrophobic group.	0	No relations to chemical properties

Students' Ability To Transfer across Molecular Representation Modes and Chemical Understanding Levels

Students' ability to transfer across the three modes of molecular representation: 3D, 2D, and textual, was examined by an assignment that required them to write molecular and structural formulas, and draw the spatial structure of a molecules. ANCOVA test indicated that students who explored 3D web-based models, received statistically significant higher scores, compared to their peers ($F_{(2,171)}$=15.04, p<0.01). These results suggest that students who learn chemistry via hands-on exploration of 3D web-based visualizations improve their ability to transfer across different modes of molecular representations.

The differences between the research groups were illustrated in the students' drawings of amino acid models. More than 60% of the students in "Experimental I" group drew amino acids correctly, unlike students in "Experimental II" group (20%) and Control group (5%). Analysis of their drawings showed that students who explored the 3D web-based visualizations on their own, drew models in a more accurate way. Generally, they drew proper angles between atoms, they differentiated between different atoms by using colors and/or proportional size, they did not misplace any atom, and their drawings included shadows to illustrate the 3D structures. Contrary to that, students who studied with teachers' demonstrations of visualizations and students from the control group, presented drawings with little or no 3D perspective

Students' ability to transfer across the four levels of chemical understanding was examined by an assignment that required them to match between the chemical and physical properties of a molecule (macroscopic level), its 2D drawing of a model (microscopic level), its structural formula (symbol level) and a processes that the molecule is involved in (process level). An ANCOVA test indicated a statistically significant difference between the three research groups ($F_{(2,\ 170)}$ =

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3.39, $p<0.05$). Post Hoc Sidak test showed that the post-questionnaire mean score of the "traditional learning" group was significantly lower than that of the other two research groups. These results suggest that in order to gain chemical understanding and be able to transfer across the four levels: macro, micro, symbol, and process, it is not enough to learn by viewing 2D drawings of molecular models in textbooks.

The results of Study 2 are further elaborated by Barak and Hussein-Farraj (*26*), indicating that the use of 2D molecular drawings or even teachers' demonstrations of 3D molecular visualizations are not sufficient for enhancing higher levels of chemical understanding and the construction of mental models. This can only be done by hands-on exploration and construction of 3D molecular visualizations.

Study 3: Integrating Visualizations into University Chemical Education

The third study was conducted in the context of university chemistry educational. Chemistry courses in higher education in Israel have traditionally been composed of lectures, exercise sessions, and laboratories. This study, introduced a new approach to chemistry learning by integrating molecular visualizations as part of the students' weekly assignments and final project. The final project was based on the constructivist learning theory, emphasizing active learning and the promotion of higher order thinking skills. Each student received a certain substance from a list of familiar substances, such as: vitamin a, nicotine, caffeine, adrenaline, TNT, DDT, etc. The students were required to use two shareware programs: MDL ISIS Draw (http://mdl-isis-draw.software.informer.com) to construct structural formulas, and ViewerLite 5.0 (http://viewerlite.software.informer.com/5.0) for the exploration and manipulation of 3D molecular models. The students were required to construct models of the assigned molecule in three representation modes, compute its molecular weight, indicate hybridization and electrical charge distribution for each carbon atom, and seek information on the Web about the daily use and function of the substance. Students from both groups spent an average of two hours per week practicing chemistry after class hours. Control students spent time on traditional problem-solving assignments; while the experimental students spent time working on their visualization projects.

Study 3 Research Questions and Participants

In order to examine the effect of web-based 3D molecular visualizations on university students' learning outcomes, the following research questions were raised: Whether and to what extent the use of visualizations effect students':

1. Conceptual understanding and argumentation skills?
2. Ability to transfer across molecular representation modes and chemical understanding levels?

The research included a representative sample of 215 freshman and sophomore students who participated in general chemistry courses. The students were divided into two groups: experimental (N = 95) and control (N = 120). All the students studied with the same instructor and the same teaching assistants. The only difference between the two research groups was the final project that the experimental group carried out, which involved an intensive use of molecular visualizations. The experimental students were actively engaged in constructing 3D molecular models, rotating them, calculating angles and measuring distances between atoms. They were applying kinesthetic-hands-on learning. Chi-Square test indicated no statistically significant differences between the research groups in respect to their academic level and gender distribution.

Study 3 Pre- and Post-Questionnaires

The pre- and post-questionnaires administered in this study consisted of three assignments. The first assignment examined students' argumentation skills in the context of chemical understanding. The second assignment was designed to examine students' ability to transfer across the three modes of molecular representation: three dimensional (3D), two-dimensional (2D), and textual. The third assignment was designed to indicate students' ability to transfer across the four levels of chemical understanding: macroscopic, microscopic, symbolic and process.

In addition to the pre- and post-questionnaires, the students' final examinations were also analyzed. The examinations were written by the chemistry instructor, containing open questions regarding the atomic theory, stoichiometry, property of gases, liquids and solids, chemical equilibrium, chemical thermodynamics, chemical kinetics, chemical bonding, and molecular orbitals. The content validity was established by the instructor, who is an experienced lecturer. The reliability of this examination is based on the observation that the examination scores were consistent with those of prior semesters.

Study 3 Findings

The findings section includes two parts. The first part presents students' conceptual understanding and argumentation skills. The second part presents students' ability to transfer across the three modes of molecular representation and the four levels of chemical understanding.

Students' Conceptual Understanding and Argumentation Skills

To investigate the effect of molecular visualizations on students' conceptual understanding, an analysis of covariance (ANCOVA) of the post-questionnaire and the course final examination scores was conducted. Findings indicated that the experimental group students received statistically significant higher scores in both the post-questionnaire and the course final examination ($F_{(1, 213)}$=57.49,

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p<0.001; $F_{(1, 213)}=5.19$, $p<0.05$, respectively). These results suggest that students who constructed and manipulated molecular visualizations improved their conceptual understanding to a larger extent compared to the control group.

The first assignment in the pre- and post-questionnaires required the use of higher order thinking skills. It tested the students' ability to analyze information about six compounds, select the best anesthetic substance and provide arguments for their choice. Given that ether is flammable and chloroform is known to cause liver damage, the students were asked to select the best alternative anesthetic and provide explanations. The scoring scheme was based on the level of students' arguments and their ability to transfer between the four chemical understanding levels: macroscopic, microscopic, symbolic and process. In their arguments, students were expected to refer to the substances' physical and chemical properties, structural formula, molecular mass, boiling point, AD_{50} (anesthetic dose), LD_{50} (lethal dose), anesthetic index, and halogen percentage.

The responses were categorized into three groups: high level arguments, partial or insufficient arguments, and no argument. Examples of students' responses are presented in Table III.

Table III. Examples of students' responses to the argumentation skills assignment

Students' responses	*Score*	*Levels of chemical understanding*
Since the halogen percentage is high, there is little chance that the carbon compound will burn when mixed with air resulting in the diffusion of O_2. Its lethal dose is very low and on the other hand, its anesthetic index is high.	3	Transfer from the microscopic to process to the symbolic level.
Due to its high boiling point, it will not evaporate in room temperature or in the patient's body. It can be injected in low concentration, because of its molecular structure.	2	Transfer from the macroscopic to the microscopic level
$CF_3CH_2CF_3$ *is a good possibility*	1	Symbol

Analyzing the students' scores in this question we found a statistically significant difference between the experimental and control groups ($F_{(1,213)}=31.08$, $p<0.001$). The percentage of the students who provided high level arguments in the experimental group was twice as much as that of the control group, while for partial arguments it was 1.4 times as much. Conversely, the percentage of students who gave no argument in the experimental group was one third of the corresponding percentage in the control group. These results suggest that the construction and manipulation of molecular visualizations enhance students' argumentation skills and chemical understanding.

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Students' Ability To Transfer across Molecular Representation Modes and Chemical Understanding Levels

Students' ability to transfer across the three modes of molecular representation: 3D, 2D, and textual, was examined by an assignment that required them to write molecular and structural formulas, and draw models. ANCOVA test indicated that students who constructed 3D molecular visualizations, received statistically significant higher scores, compared to their peers ($F_{(1, 213)}$=26.68, p<0.001). Findings indicated that the integration of the 3D molecular visualizations into the general chemistry course final project was the source for the difference in the students' ability to transfer across the three modes of molecular representation.

The analysis of the students' drawings of molecular models indicated that more than 70% of the experimental group students drew correct models, compared to only 50% of the control group students. Space-filling model was the most popular representation among the experimental group, accounting for 70% of the drawings. Among the control group, the ball-and-stick model was the most popular representation, accounting for 46% of the drawings. Experimental group students were thorough and presented details such as non-bonding electrons, tetrahedral angles, and atoms in front or behind the central atom. Experimental group students used various sizes and colors to differentiate between the carbon, oxygen, and hydrogen atoms in the molecule. In contrast, most control group students drew the models as if the atoms were connected at 900 angles and their sketches were less meticulous about details, proportions, and colors.

Students' ability to transfer across the four levels of chemical understanding was examined by an assignment that consisted of four parts, each relating to a chemical understanding level: a. identifying the substances properties (macroscopic level), b. identifying the correct model (microscopic level), c. recognizing the correct formula (symbolic level), and d. completing and balancing chemical equations (process level). An ANCOVA test indicated a statistically significant difference between the two research groups ($F_{(1, 213)}$=40.12, p<0.001); showing that the post-questionnaire mean score of the students that constructed molecular visualizations was significantly higher than that of the control group.

The results of Study 3 have been further elaborated by Barak and Dori (*8*), indicating the positive outcomes of project-based learning with an extensive use of 3D molecular visualizations. These results suggest that while constructing and manipulating computerized molecular models, students are likely to develop chemical understanding as well as argumentation skills.

Summary and Discussion

This chapter describes three studies with one similar objective: to examine the effect of web-based 3D molecular visualizations on students' learning outcomes; centering on five cognitive abilities: a. conceptual understanding, b. transfer across four levels of chemical understanding, c. transfer across three modes of molecular representations, d. model drawing, and e. explanation or argumentation. The findings in all three studies suggest that in order to enhance the construction of mental models, students should be actively engaged in learning via 3D dynamic visualizations. Following Mayer's cognitive theory (*11*), our findings can be explained by the fact that while constructing and manipulating molecular visualizations, the students use two cognitive channels: auditory-verbal and visual-pictorial. In the auditory-verbal channel, students process narration and voices, organizing them into cognitive schemes. In the visual-pictorial channel, students process visualizations (graphs, photos, videos), organizing them into cognitive images. Instructional conditions that promote the integration of both processes are most likely to result in meaningful learning (*11*).

In addition to the two cognitive channels described by Mayer (*11*), our findings indicated that there in a need for a third cognitive channel: the kinesthetic-hands-on channel, in which students are actively engaged in manipulating and constructing the 3D molecular visualizations. Findings indicated that the use of drawings presented in textbooks or even in teachers' demonstrations of 3D visualizations, are not sufficient for enhancing higher levels of cognitive abilities. In all three studies, students that were actively engaged while learning with visualizations, received higher grades compared to their peers in the control groups. In study 1, the elementary students watched the 3D animations in computer clusters while answering questions or carrying out assignments. In study 2, the high school students manipulated the 3D visualizations by rotating them and changing representation modes. In study 3, the university students constructed 3D molecular models and calculated angles and distances between atoms.

The kinesthetic-hands-on channel supports the organization of newly acquired information into scientifically correct mental images. Consequently, while learning chemistry, students should be actively engaged in constructing molecular models, rotating them, calculating angles, measuring distances between atoms, and manipulating different types of molecular representations. These actions indicated a positive effect on students' ability to transfer across the four levels of chemical understanding: macro, micro, symbol, and process, and three molecular representation modes: 3D, 2D and textual (*8*, *18*). Indeed, molecular visualizations should combine text, sound, and dynamic graphics, for supporting the three learning styles: visual, auditory, and kinesthetic, and for simultaneous use of three senses: sight, hear, and touch. Similar to other studies, our findings indicate that a multimedia-based learning environment promote students' learning outcomes, (*10*, *12*). Some learners prefer visual presentations, some prefer auditory processing, and others hands-on activities; therefore, effective visualizations should involve multimedia: text, sound (narration and/or music), and touch.

In the past two decades, research has indicated that the use of visualizations contributes to students' spatial abilities (*13*, *19*), learning achievements (*12*, *19*), conceptual understanding (*8*, *16*, *17*), and motivation to learn science (*20*). Nowadays, chemistry educators no longer ask "whether visualizations improve learning", but rather "what are the conditions in which visualizations can be most efficient for learning". Based on the three studies, it is suggested that visualizations should be relevant to the curriculum and well integrated throughout

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the learning process. They should be a central part of the learning materials, accompanied by supplementary activities that emphasize scientific thinking. Visualizations should also be explored gradually and recurrently; first, to the entire classroom for initiating class discussions on related scientific phenomena; then, it should be explored in small working groups for enhancing knowledge sharing; lastly, visualizations should be explored and manipulated individually for promoting scientific thinking. Our studies indicated that these learning processes support the creation of mental representations of scientific concepts, while enhancing students' explanation abilities, argumentation skills, and motivation to learn science (*8*, *20*).

As indicated above, visualizations can enhance various cognitive processes that are reflected in students' learning outcomes. In addition to Mayer's cognitive theory (*11*), there is another possible explanation for these positive results. This explanation relates to the idea that external visualizations can enhance existing images or substitute for internal visualizations. An external visualization can provide supplementary information, and thus assist people with low visualization ability in creating or restructuring their mental models (*7*). In the studies described above, this trait was mainly indicated in students' drawings of molecular models. Students who explored and manipulated 3D molecular visualizations, whether in elementary, high-school, or higher education, drew all the essential atoms, drew relatively accurate angles, used colors to differentiate between the atoms, and in some cases used shadows and proportional sizes to illustrate the 3D structures. The students' drawings provided proof for the reciprocal nature of external and internal visualizations. By exploring 3D molecular visualizations (external visualizations), the students improved their mental models (internal visualizations), indicated by drawing better and more accurate molecular models (external visualizations).

Some claim that visualizations may carry a potential for misconceptions and hinder meaningful learning (*21*). The three studies presented above indicate otherwise; providing that the visualizations are well-structured, used when learners cannot visualize without them (*21*), and when learners can construct and manipulate the computerized models on their own (*9*). Indeed, among the many advantages of using advanced technologies in chemical education, web-based visualizations are significantly important for helping students' "see the unseen", thus improving their chemical understanding.

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Chapter 12

The Effect of Student-Constructed Animations versus Storyboards on Students' Mental Rotation Ability, Equilibrium Content Knowledge, and Attitudes

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This study evaluated how general chemistry students' mental rotation abilities, knowledge of physical and chemical equilibrium, and attitudes were affected by the use of one of two different visualization assignments. One class created storyboards with paper and pencil and the other created computer animations with the ChemSense computer program. Both classes showed significant gains in mental rotation abilities and content knowledge, but there was no difference between treatments. No significant differences in content knowledge scores were found between the males and females in the study. However, male students significantly gained in mental rotation abilities over females. In the attitude survey, students believed the activities helped them learn equilibrium content. Both males and females regardless of treatment indicated that the visualization assignments were generally easy as opposed to hard to construct, but females indicated this fact significantly more so than the males. Instructors should be encouraged to use either method to increase mental rotation ability and help with equilibrium understanding.

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Background

Johnstone proposed that chemistry had three basic components: macroscopic, submicroscopic, and representational (*1*). Macroscopic chemistry studies the visible world around us. The submicroscopic component of chemistry describes matter in terms of particles, including their composition and behavior. Representational chemistry is the use of symbols in variables and chemical formulas. This study focuses on the submicroscopic or particulate level of chemistry.

Many high school and college students have trouble understanding scientific concepts and visualizing objects in three-dimensions. A number of researchers have proposed that many student misconceptions in chemistry result from the inability to visualize particles or the faulty visualization of particle behavior (e.g., (*2*, *3*)). Students of chemistry need to be able to correctly visualize atoms and how they are bonded together in three dimensions. José and Williamson (*4*) analyzed the outcomes of a visualization workshop held through the National Science Foundation. They found that the expert participants of the workshop endorsed and proposed the use of visualization techniques in the classroom to promote particle understanding. These participants included chemists, software developers, cognitive scientists, and chemical education researchers.

Previous studies have analyzed different methods of helping students learn how to visualize chemical and physical processes. Sanger (*5*) investigated the understandings of college students in a general chemistry course. He found that: "students who received instruction that focused on the characteristics of pure substances and mixtures at the microscopic level were more likely than students who received traditional instruction at the macroscopic level to correctly identify particulate drawings of liquids, pure compounds, heterogeneous mixtures, homogeneous mixtures, elements, and compounds. (pp765-766)" He concluded that instruction using particulate drawings and computer animations are very useful in helping students correctly answer questions about chemical processes.

Visualization can be a powerful tool to help explain chemical processes and properties. Williamson and Abraham (*6*) found that short duration animations used during lecture in a 2-week unit of study on gases, liquids, and solids significantly improved general chemistry students' conceptual understanding. These authors repeated the study with a unit on reaction chemistry. The finding of significant improvements in conceptual understanding for the treatment group that received instruction using particulate animations was the same. Sanger and Badger (*7*) studied how to best communicate the concepts of molecular polarity and miscibility. They found that college students exposed to computer animations and electron density plots gained a better understanding of molecular polarity and intermolecular forces.

Student-generated drawings/animations can be used to evaluate student understanding, although they may be hard to interpret/grade (*5*). One way to ascertain student understanding is to ask students to draw their ideas. Harrison & Treagust (*8*) used student drawings to evaluate student understanding. They proposed that students should receive instruction with visualization techniques appropriate to their cognitive ability; however, instructors should gradually

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challenge students to use more abstract models. Further, multiple models should be used in instruction. A case study was used to explain how the systematic use of models improved a high school chemistry students' understanding of atoms and molecules.

Milne (*9*) reported the effects of using index cards to model chemical reactions. Students at the secondary level were given 20 index cards to model a chemical reaction by creating a "flip book." This allowed students to visualize the motion in a chemical reaction, as well as the kinetic and stoichiometric properties of reactions. He found that students became very engaged while they created storyboards (in the form of note cards) to simulate chemical reactions. Storyboards were proposed as an effective way to actively engage the students and to teach chemical reactions, even though the study did not investigate the impact on content knowledge.

There is some evidence that student creation, rather than just presentation, of models can lead to enhanced understanding. With computer programs, students can produce their own animations. Schank and Kozma (*10*) investigated ChemSense, a molecular drawing and animation tool. In one of the reported experiments, high school students who used ChemSense had a significant improvement in their understanding of connectivity and geometry of molecules from pre- to post-test. Also, a positive correlation was found between the number of drawings and animations produced in a 3-week unit and the chemical correctness of the animations produced. From the video recordings of students working on their animations, the authors propose that students were able to better represent chemical phenomena at the particulate level as a result of the planning and consideration of what to put in each frame of the animation. Students were more focused on aspects of the chemical phenomena that they would not normally consider, including the geometry, the sequence of steps, and the dynamic nature of chemical reactions

While storyboards and animations may help student understanding, previous research has also found a link between having good spatial abilities and performing well in chemistry courses. Spatial abilities include a number of visuo-spatial abilities, of which mental rotation ability, the ability to rotate in three dimensions, is a major component (*11*). In organic chemistry courses, students with high spatial abilities as measured by a mental rotation test and a hidden shape test did significantly better on questions which required problem solving skills, but no different on rote-memory questions (*12*). Further, high spatial students drew molecules in three dimensions without being prompted when answering questions and were more likely to get problems correct (*12*). In a similar study, students who score higher on the same spatial ability tests are more likely to perform well in general chemistry courses (*13*). This suggests a link between spatial abilities and performance in chemistry, at least during the first two years of college chemistry. Finally, it has been shown that there is a significant lack of spatial abilities amongst college students regardless of gender (*14*), and that there is a need to address this problem.

This study investigated two different means to foster student understanding of particles (student-constructed storyboards and animation) and to compare the effectiveness of the two treatments when using the concepts of physical and

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chemical equilibrium. It also focuses on mental rotation abilities and performance on a chemistry content quiz dealing with these concepts. A number of researchers have found that students lack a conceptual understanding of equilibrium (e.g. (*15*)). In this study, college students were assigned projects (either to construct storyboards or animations) to determine their understanding of the concepts of chemical and physical equilibrium. When students are assigned a project, they must be creative, ask questions, and take responsibility for their own learning. Students were required to construct a mental model of a process in their minds and express it. Constructivism is the theoretical frameworks behind this style of teaching/learning.

In constructivism, the student-learners are guided by a facilitator, but students take the bulk of the responsibility for their own learning (*16*). Bodner (*17*) states that "[k]nowledge is constructed in the mind of the learner." He also makes the case that a teacher should facilitate learning, and not simply attempt to transfer knowledge into the minds of the students. The Constructivist model of learning is greatly influenced by the work of Jean Piaget. Piaget believed that we can learn about another's mental mindset by observing this individual's behavior. He also stated that a person's intellectual growth is linked to his physical and social environment. Finally, he used the fact that humans are a biological species as an influence to theorize that we are motivated to grow and change by a process of "organization and adaptation" (*18*). Piaget has had a profound impact on educational research (*19–21*). The philosophy of Lev Semenovich Vygotsky also has had an influence on constructivism. Vygotsky believed in cooperative learning and that a student will learn with instructional help. Every learner has a Zone of Proximal Development (ZPD), which is the gap between what the learner knows and what they are capable of learning with help. With time, the learner will be able to perform certain tasks without assistance (*22*).

The purpose of this study was to investigate the effectiveness of two visualization techniques, student-constructed storyboards and animations. The goal was to analyze how these techniques can help students better understand equilibrium concepts and better visualize objects in three dimensions.

Research Questions

The specific research questions are:

1. How are general chemistry students' mental rotation ability and equilibrium content knowledge affected by the construction of computer animations or the construction of storyboards?
2. What are students' attitudes toward drawing three-dimensional molecules with computer animations or with paper and pencil?

Research Procedures

This research project involved two college classes of second semester general chemistry at a large southwestern university. Each class contained approximately

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300 students. The first activity given to the students was a pre-test, which occurred before any instruction on equilibrium was given in the lecture or the laboratory portions of the courses. This test contains seven multiple-choice questions, each one related to equilibrium, and was given in class as a quiz for a quiz grade. These questions were conceptual based, and the math required was minimal. Scores on the content pre-test ranged from 0-7. A few sample questions are included in Table 1.

Table 1. Sample Pre-test Questions

3. For the reaction A(g) + B(g) ⇆ C(g) + D(g), K = 0.001. Which statement best describes this reaction at equilibrium? a) There is much more A and B than C and D. b) There is much more C and D than A and B. c) There are equal amounts of A, B, C, and D. d) The reaction has gone to completion; all of the A and B have been depleted.
5. Which of the following is ALWAYS TRUE about chemical equilibrium? a) At equilibrium, the chemical reaction stops. b) If K = 10, then the forward reaction rate is faster than the reverse reaction rate. c) The equilibrium constant is independent of reactant concentration. d) At equilibrium, the concentrations of all reactants and products are the same.
7. The following reaction, 2A(g) ⇆ B(g), has concentration of A and B as 2 M and 1 M, respectively. If the equilibrium constant is 0.50, what can be said about this reaction? a) The reaction is at equilibrium. b) The reaction is not at equilibrium, and more products will be formed until equilibrium is established. c) The reaction is not at equilibrium, and more reactants will be formed until equilibrium is established. d) The reaction is not at equilibrium, and the reaction will shift until the concentrations of the reactants and products are the same.

The students were then assigned to take an online assessment, which tested their mental rotation ability. The Vandenberg Mental Rotations Test, Vandenberg Test, or MRT is widely used and requires students to answer questions related to the rotations of three-dimensional shapes. Vandenberg and Kuse (*23*) reported that this test has internal consistency and reliability between taking the test multiple times, and differences in results between males and females. Each question provides a three-dimensional object in picture form and asks for the student to indicate which two of the four choices illustrate the same object, which has been rotated in some manner. There are 20 total questions (each worth two points), and the test is split into two sections of 10 questions each. Each student was given three minutes to complete the first half and another three minutes to complete the second half. The computer programming did not allow the student to return to a previous page and moved forward once three minutes of time had passed. There are two correct answers to each question. If a student selects only the two correct choices for a question, two points are awarded. If a student selects one correct choice and one incorrect choice, zero points are awarded. If only one correct choice is selected and no others, one point is awarded. Finally, if a student does not answer a question, no points are awarded.

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Immediately after the Vandenberg Test was completed, each lecture class of students was asked to create a model of a physical equilibrium via different means. A coin flip was used to determine the treatment (storyboards or ChemSense animations) assigned to a lecture class. Students in each lecture class were divided into groups of 24 for laboratory. Students were assigned a physical system to model from a list of 24 possibilities. They were later assigned a chemical reaction to model from a list of 24 possibilities. For example: One student could be assigned to model the equilibrium established between liquid and gas phases of H_2O ($H_2O(l) \leftrightarrows H_2O(g)$) and the equilibrium involved with the chemical reaction $H_2(g) + I_2(g) \leftrightarrows 2HI(g)$. With the pool of 24 physical and 24 chemical equilibria, every student in a laboratory section was assigned a different physical and chemical process. The assignments were randomized such that the physical equilibrium was not paired with the same chemical equilibrium, so students in the second laboratory would not have the same pairings as students in the first laboratory. One assignment may be more difficult than another, but each laboratory section was assigned the same set of problems and the averages of the scores on these assignments were analyzed. The assignments for the two treatments (storyboards or ChemSense animations) were from the same list of choices and done in the same manner. All of the students were given a week to perform the activity for physical equilibrium and a second week to complete a chemical equilibrium.

One lecture class (broken into 12-13 laboratory sections) was assigned to create two animations that simulated the two different assigned equilibria using the ChemSense computer program (*10*). ChemSense had been used previously at this institution. Students in first and second semester general chemistry had been asked to use it to model chemical reactions that go to completion during six previous semesters. It should also be noted that ChemSense is easy to use and has been used as a tool in education research as previously discussed (*10*, *24*). A short, two-page tutorial guide that had been provided to students in these past semesters was also used in this study. The tutorial walks students through the construction of a trial animation of hydrogen gas plus oxygen gas forming water. Students were told that their animation should contain at least 10 frames and were given the grading rubric (see Table 2).

Table 2. Scoring Rubric for Both Storyboards and ChemSense animations

8 pts	At least 10 frames long, 1 pt Chemically correct, 2 pts • Atoms are correctly bonded together, 1 pt • Atoms are labeled correctly, 1 pt Equilibrium illustrated correctly, 5 pts • The forward and the reverse processes must be illustrated, 2 pts • Once equilibrium has been established, there must be reactant molecules changing into products at the same rate that product molecules are changing into reactants, 3 pts

The other lecture class was required to create storyboards to model the assigned physical and chemical equilibria. Students were told that a storyboard is a series of still pictures to mimic motion. Further they were told that their storyboard should contain at least 10 pictures and were given the grading rubric. Table 2 provides the rubric (which was made available to all students) for grading the storyboards and ChemSense assignments. A student must have the correct proportion of atoms drawn for the molecule in order to receive full credit for the chemically correct portion of the rubric. Also, the forward and reverse processes in equilibrium must be illustrated clearly.

Once the students had all completed their assignments of modeling a physical and a chemical equilibrium, the students were given the post-test (as a quiz grade) in the lecture class. The post-test is similar to the pre-test, but contained different questions related to equilibrium. There were seven multiple-choice questions on the post-test, conceptually based, and therefore the scores ranged from 0-7. The post-test also asked students questions about their attitudes toward drawing molecules with the use of ChemSense or with pencil and paper, using one semantic differential question and five open response questions. Finally, students were given the Vandenberg Test again, which was again offered online. The second iteration of the mental rotations test was given about five weeks after the first iteration, to help negate gains from just retesting. The order was such that content pre-test, the first Vandenberg Test, the equilibrium unit of study, and the post-test were followed by the second mental rotation test.

The instructor routinely gave the Test of Logical Thinking (TOLT) to her classes as a quiz near the beginning of the course to help gauge the level of mathematics instruction needed. The TOLT tests one's ability to understand control of variables, proportionality, combinations, correlation logic, and probability logic. The TOLT has a high reliability (*21*, *25*) as students must get both the correct answer and reason for their answer in order to receive credit for an item. There are ten total questions on the TOLT; therefore a student can earn a score of 0-10.

Quiz credit was offered for the TOLT, pre-test, post-test, and both administrations of the Vandenberg test (which will from this point be referred to as MR ability I and MR ability II). The two classes required 11 quizzes (at 4 points each), but typically 19-20 were given throughout the semester. Quiz credit constituted 44 points out of a total 1000 points for the course. The classes also required 16 points of special assignments, which can include projects, seminar summaries, take-home worksheets, etc. Eight points of special assignment credit were offered for each of the two visualizations produced (ChemSense or storyboards). Students were asked to participate in the study by releasing their grades for the TOLT, pre-test, post-test, MR ability I and MR ability II. The storyboard class had 143 students participate in the research project; while the ChemSense animation class had 157 students participate.

After the students took the Pre-test, TOLT, and MR ability I, they were exposed to the specific equilibrium material in lecture, laboratory, and in the assignments of ChemSense and storyboards. They obviously learned from all of these sources. The purpose of this study is to analyze the value added, if any, when students use electronic (ChemSense) or paper and pencil (storyboards) means to study chemistry material. The data from the TOLT was analyzed to determine group equivalency. An analysis of the pre-test vs. the post-test scores was done to determine if learning has occurred for each group. Also, an analysis between the gains for each group investigated any differences on content learning between the two treatment groups. Similar analysis of the mental rotation ability data determined if there have been any changes pre- to post- within each group and if there are any changes, if these differ between the two treatment groups. Also, the students' attitudes between the two treatment groups were compared and contrasted. As a series of two-tailed t-tests are required for all these analyses, a MANOVA was also used to help control error.

Results

Table 3 reports the average scores of both groups on the TOLT, pre-test, and post-test, in addition to their average age. Age was calculated by asking the students to enter their birthdays online when they took the Vandenberg Test. The TOLT is scored out of ten points, and the pre- and post-tests are both scored out of 7 points. The students took the Vandenberg Test twice, MR ability I first and then MR ability II, which are reported in Table 3. The second time the students took this test, they had completed all of the storyboard or ChemSense assignments. The Vandenberg Test is scored out of 40 points.

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Table 3. Means and Standard Deviations for Age, Reasoning Ability, Content Tests, and Mental Rotation Abilities

	Storyboard (n = 143)	***Animation (n = 157)***
	Mean (SD)	*Mean (SD)*
Age	19.19 (1.67)	18.90 (0.60)
TOLT	7.84 (1.89)	7.47 (2.01)
Content Pre-test	2.52 (1.22)	2.40 (1.27)
Content Post-test	4.41 (1.43)	4.42 (1.48)
Mental Rotation Ability I	15.85 (6.48)	15.81 (8.12)
Mental Rotation Ability II	20.32 (8.68)	20.05 (9.64)
Physical Equilibrium Grade	5.60 (2.02)	6.13 (1.79)
Chemical Equilibrium Grade	5.12 (2.08)	6.06 (2.14)

Each equilibrium assignment was graded out of eight points. The majority of the points were given for depicting a conceptual understanding of equilibrium. Table 3 also summarizes each group's average scores on the physical and chemical equilibrium. Each assignment was scored by the second author. These scores were randomly checked by another rater who used the same rubric, with a 94% inter-rater agreement.

There was a total of six questions on the attitudinal survey given with the post-test. The mean was calculated for the first survey question. This 7-point, semantic differential question asked students to rate the visualization assignments' difficulty level. Table 4 shows these data.

Table 4. Scores on the Semantic Differential Question Given on the Survey

Question	***Storyboard (n = 143)***	***Animation (n = 157)***
	Mean (SD)	*Mean (SD)*
1. How easy was it for you to produce the assigned visualizations? Please circle only one number. Easiest 1 2 3 4 5 6 7 Hardest	3.34 (1.32)	3.17 (1.20)

Questions 2, 3, and 4 asked the students to answer yes or no and to explain. Some students did not choose yes or no, so were coded as undecided. The tallies of the yes (Y), no (N), and undecided (U) responses are reported in Table 5. The Animation Group had a higher fraction of students respond favorably (indicating yes) to all three of these questions than the Storyboard Group.

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Table 5. Questions Requiring Both an Answer and an Explanation on the Survey

	Storyboard (n = 143)			***Animation (n = 157)***		
Question:	*Y*	*N*	*U*	*Y*	*N*	*U*
2. Did producing the required visualization help you learn chemistry content (yes or no)? Please explain.	95	46	2	111	46	0
3. Did producing the required visualization help you to better visualize objects in three-dimensions (yes or no)? Please explain.	75	68	0	102	55	0
4. Were the benefits of producing the required visualization worth the time it took to produce them (yes or no)? Please explain.	79	58	6	94	60	3

There were five opportunities for open responses on the survey. Questions 2-4 in addition to asking for the yes or no responses, which were reported in Table 5, also gave each student the opportunity to explain the response. Questions 5 and 6 allowed students express his/her point of view about the visualization assignments when asked what was the best part and what was the worst part of producing the required visualization. Examples of some responses to all these questions are provided in Table 6. These examples are representative of both the positive and negative comments given.

Analysis

Both the Animation and Storyboard Group averaged above 7 on the TOLT. In the 1981 initial validation study, college students enrolled in science courses scored an average of 4.4 on the TOLT (*21*). In another study, two groups of college students enrolled in a junior-level quantitative analysis course scored above 8 on this test (*25*). It is clear that both groups in this study understand important mathematical concepts and can think logically.

A MANOVA was performed to determine if the two classes were statistically equivalent based on a variety of dependent variables. Table 7 reports the results for their TOLT scores. There is no statistical difference between the two groups with respect to their TOLT scores.

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Table 6. Responses to the Open Questions Given on the Survey

2. Did producing the required visualization help you learn chemistry content (yes or no)? Please explain.	
Storyboard Group	***Animation Group***
• Yes, [it] reinforced understanding of how molecules behave in trying to achieve equilibrium. • No it did not. I already understood equilibrium. • Yes, I could see how the reaction progressed in both directions.	• No, I already understood the concepts. • Yes, had to think for ourselves how reaction occurred. • No, I already knew what equilibrium meant, doing the animation was a pain. • Yes, it helped me understand equilibrium and its relationship with reactants and products.
3. Did producing the required visualization help you to better visualize objects in three-dimensions (yes or no)? Please explain.	
Storyboard Group	***Animation Group***
• Yes, because I am a visual learner. • No, the drawings were two-dimensional.	• Yes, it did help me visualize it better. • No, I have never been good at visualizing 3D objects.
4. Were the benefits of producing the required visualization worth the time it took to produce them (yes or no)? Please explain.	
Storyboard Group	***Animation Group***
• Not at all. I could have visualized it in my head. • It didn't take too long and it helped me to see the reaction.	• Yes, because they did not take very long. • No, it took a long time for me.
5. What was the best part of producing the required visualization?	
Storyboard Group	***Animation Group***
• It was better than having to write a paper to try to explain it. • Quick and easy, not just homework but something different.	• Making a chemistry movie was kind of fun. • Watching the animation once it was done.
6. What was the worst part of producing the required visualization?	
Storyboard Group	***Animation Group***
• It was time consuming and I'm bad at art. • Filling in 10 slides, didn't need 10.	• The time it took to make. • Program slightly confusing and it took a while to get the molecules to do what you wanted them to do.

Table 7. MANOVA Results between the Storyboard and Animation Groups

	p-value
Age	0.0451[a]
TOLT	0.0978
Content Pre-test	0.3914
Content Post-test	0.9299
Mental Rotation Ability I	0.9652
Mental Rotation Ability II	0.7945
Physical Equilibrium Grade	0.0162[a]
Chemical Equilibrium Grade	0.0001[a]

[a] significant difference, $p < 0.05$

The Storyboard Group was statistically significantly older ($p = 0.0451$) than the Animation Group. However, no changes in the results were found when age was used as a covariant. For the TOLT, content and MR ability measures taken by the two groups, there was no significant difference between groups. There was, however, a significant difference in the grades received on the equilibrium projects ($p = 0.0162$, $p = 0.0001$). The Animation Group scored significantly higher in modeling the physical and chemical equilibrium processes than the Storyboard Group. It is not clear why there should be a difference in scores on the equilibrium assignments. When looking at the grading rubric in Table 2, there does not appear to be a bias.

Table 8 reports the comparisons between changes within the groups on content and mental rotation ability. Content knowledge is gauged with the administrations of the pre-test and post-test (see Table 3). There is a significant gain in understanding in course content; hence there was a rise in scores for both groups between the pre- and post-tests. Additionally, MR ability II is statistically significantly higher than MR ability I, regardless of the treatment group. Both groups increased in content knowledge of equilibrium and increased in mental rotation ability during the equilibrium unit of study, which lasted about 4 weeks and was between the pre- and post- content tests.

Table 9 reports each treatment group by gender. Within the Storyboard Group, there was a significant difference in comparing MR ability II and survey question #1. Males scored significantly higher on MR ability II. Females believed that the task of producing the assigned visualization was easier than the males believed. Within the Animation Group, a significant difference was observed when comparing the results for MR ability I and MR ability II. Males scored significantly higher than females on both of these tests. Also, there was a significant difference in the responses to survey question #1. Females in each treatment group indicated that producing the visualization assignment was an easier task more so than the males in the group.

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Table 8. MANOVA Results for Changes in Content and Mental Rotation Ability

	p-value
Content Pre-test to Content Post-test	
Storyboard Group	<0.0001[a]
Animation Group	<0.0001[a]
Total	<0.0001[a]
MR Ability I to MR Ability II	
Storyboard Group	<0.0001[a]
Animation Group	<0.0001[a]
Total	<0.0001[a]

[a] significant difference, $p < 0.05$

Table 9. MANOVA Results by Gender within each Group

	Storyboard Group *p-value*	***Animation Group*** *p-value*	***Total*** *p-value*
Age	0.3958	0.8279	0.4125
TOLT	0.5223	0.1093	0.0603
Content Pre-test	0.5934	0.5439	0.6762
Content Post-test	0.2118	0.1489	0.0635
Mental Rotation Ability I	0.2491	0.0005[a]	0.0002[a]
Mental Rotation Ability II	0.0119[a]	0.0002[a]	<0.0001[a]
Physical Equilibrium Grade	0.1767	0.5886	0.1039
Chemical Equilibrium Grade	0.4576	0.4328	0.6272
Survey Question #1	0.0247[a]	0.0225[a]	0.0016[a]

[a] significant difference, $p < 0.05$

For the total study population, composed of both treatment groups, there were significant differences for MR ability I, MR ability II, and survey question #1. Males scored significantly higher than females in both iterations of the MR Abilities Test. For survey question #1, the means were 3.42 (SD=1.28) and 2.94 (SD=1.17) for the males and females, respectively. Once again, females indicated that the task of producing the assigned visualizations was an easier task than the males indicated. Although the females thought the visualizations were easier to produce, the mean for the males was still below the neutral midpoint of 4.

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The content gain was found by subtracting the pre-test from the post-test. The mental rotation ability gain was found by subtracting MR ability I from MR ability II. These gains were investigated to see if there was a difference in the gain by gender, and the results are reported in Table 10.

Table 10. MANOVA Results in Comparing Changes in Content and Mental Rotation Ability by Gender

Content Gain (Content Post-test minus Pre-test)	***Males Mean (SD)***	***Females Mean (SD)***	***p-value***
Storyboard Group Males to Females	2.16 (1.65)	1.73 (1.77)	0.1608
Animation Group Males to Females	2.19 (1.63)	1.94 (1.62)	0.3872
Total Males to Females	2.12 (1.66)	1.86 (1.71)	0.1995
Mental Rotation Ability Gain (MR Ability II minus MR Ability I)	***Males Mean (SD)***	***Females Mean (SD)***	***p-value***
Storyboard Group Males to Females	6.12 (8.01)	3.62 (5.35)	0.0506
Animation Group Males to Females	5.11 (7.11)	3.90 (7.24)	0.3317
Total Males to Females	5.65 (6.19)	3.62 (7.58)	0.0184[a]

[a] significant difference, $p < 0.05$

The mean of the difference between the post-test and the pre-test is a positive number for both males and females. Also, for males and females, the mean of the difference between MR ability II and MR ability I is a positive number. However, no significant difference was found in these gains when comparing males and females, except when the total number of males and females were compared in regards to their respective gains in mental rotation abilities. Males gained significantly more in mental rotation abilities than females in this study. The averages for the pre-test, post-test, MR ability I, and MR ability II for the total males and females are provided in Table 11.

Paired t-tests were performed comparing the results, by gender, of the content pre-test to the post-test, as well as comparing MR ability I to MR ability II. Within the Storyboard and Animation Groups, males scored significantly higher on the post-test than the pre-test (p-values < 0.0001). Also, males, within each group, scored significantly higher on MR ability II than MR ability I (p-values < 0.0001). Finally, the total male population significantly raised their scores from the pre-test to the post-test and from MR ability I to MR ability II (p-values < 0.0001).

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Table 11. Averages of Content Tests and Mental Rotation Ability Tests for Males and Females

	Males mean (SD) (n = 108)	*Females mean (SD) (n = 192)*
Content Pre-test	2.50 (1.15)	2.44 (1.29)
Content Post-test	4.62 (1.44)	4.30 (1.45)
MR Ability I	17.95 (7.57)	14.63 (7.00)
MR Ability II	23.60 (9.16)	18.25 (8.64)

The exact same results for the females resulted from the paired t-tests. Females significantly raised their scores from the pre-test to the post-test and from MR Ability I to MR Ability II within each group and when the total female population was considered (p-values < 0.0001). It is clear that both males and females of this study gained in equilibrium content knowledge and in mental rotation abilities.

The three survey questions that required yes-no answers listed in Table 5 were analyzed using a chi-squared test. The undecided responses were combined with those that responded negatively. Using the idea that we expect no differences between the Storyboard and Animation Groups, we used a theoretical probability of an even distribution. Using these expected values, all three questions were significantly different ($p < 0.05$) between the two groups.

Discussion

The first research question was: How are general chemistry students' mental rotation ability and equilibrium content knowledge affected by the use of computer animations or the use of storyboards? The students gained in their mental rotation ability during the length of the research project. Both groups significantly improved their mental rotation ability scores; however, there was no difference between treatment groups. There was a gender effect for the total study population. It is interesting to note that males scored higher than females on both iterations of the Vandenberg Test. This result fits with the findings in the literature that males typically have a better ability to spatially-visualize objects in three dimensions. Barke (*26*), for instance, reported that males score higher on spatial ability tests than females of the same age. His study focused on students in 7th through 9th grades. For the total sample of this study, the gains in mental rotation abilities for males were significantly higher than the gains for females. Vandenberg and Kuse reported similar findings in their work with college students (*23*). Females, in both treatment groups and as a whole, significantly gained in mental rotational abilities from their pre-test to their post-test, which is consistent with previous research (*27*).

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It is clear that students in both groups gained in content knowledge after being assigned to model two different processes, one physical and one chemical. During this time, they were also exposed to course material from the lecture and lab portions of the course, so the increase in understanding cannot be attributed to the visualization assignments alone. However, both groups had similar content gains. It does not seem to matter which method is used (computer animation or storyboard). It is interesting to note that in survey question #2, the majority of both treatment groups believed the visualization assignments helped them learn chemistry content.

It is unclear as to why the Animation Group scored significantly higher than the Storyboard Group on both equilibrium projects. On examining the rubric for grading the visualization project, no bias in favor of the Animation Group could be found. It could be that college students are more comfortable with a computer interface than using traditional pencil and paper. No evidence was found in this study suggesting that college students have a better ability to use a computer interface than pencil and paper. The ChemSense software is easy to use, and very little effort is needed to model a molecule moving, shifting, and having its bonds break and reform. ChemSense has features (such as labeling an atom automatically) that could provide students an advantage over the ones who were assigned to create a storyboard. In the rubric, one point was given for labeling the atoms correctly, so this might explain the difference.

The visualization assignments resulted in uncovering a number of student misconceptions, regardless of treatment. These misconceptions are similar to those reported by others (*15*). Some students would depict the reactants all going to products, then remaining static. While others would show the reactants going to all products, then the products going back to all reactants. It could be that they were misunderstanding the term 'reversible.' Some students would show half of the reactants going to products, then remaining static with an equal mix of products and reactants.

There was one observation that may explain the similarity of the two treatment groups. Many students in the Storyboard Group made flipbooks from their static pictures without any instructions indicating this was a possibility. The Storyboard Group was told: "A storyboard is a series of still pictures that mimics motion. Please draw each one of these pictures on a 3 inch by 5 inch note card. Also, please have your story board be no shorter than ten pictures." We believe that the process for making the pictures for the storyboard was not very different from the process needed to construct a frame for the ChemSense animation. Figure 1 depicts a sample storyboard.

The second research question was: What are students' attitudes toward drawing three-dimensional molecules with computer animations or with paper and pencil? For both treatment groups (Storyboard and Animation), students believed that the assignment was relatively easy. For both groups, the means of survey question #1 were less than the midpoint of 4, which indicates that they believed, as a whole, that the assignments were easy, rather than hard to complete. Also, both males and females indicated the ease of producing the assignment with an average below 4. There was only one gender effect in the attitude survey. According to their responses to survey question #1, females believed that producing the equilibrium assignments was an even easier task than did the males of this study.

There were some interesting comments made on the other survey questions. Some students believed that the assignment was a worthwhile exercise, and some believed that it was not. It is interesting that some students commented that they enjoyed the assignment because it was different than what they are used to in a college science course. It seems to be a rewarding experience for them to participate in an alternate assignment from the normal routine of doing online homework and taking tests. Finally, some students completed the assignment in a short period of time, according to their comments, and others believed that it was a time-consuming task. The Animation Group seemed to answer more favorably to the attitude questions that asked for yes or no responses (Table 5). It is unclear as to why the Animation Group would believe to a greater extent that this project helped them to learn chemistry content and to visualize objects in three-dimensions, plus was worth the time. More of the students in the Animation Group believed the animations helped them learn content and that the MANOVA tests showed that the students in the Animation Group did learn more chemistry content (i.e., their perceptions were matched by the analysis of their post-test responses).

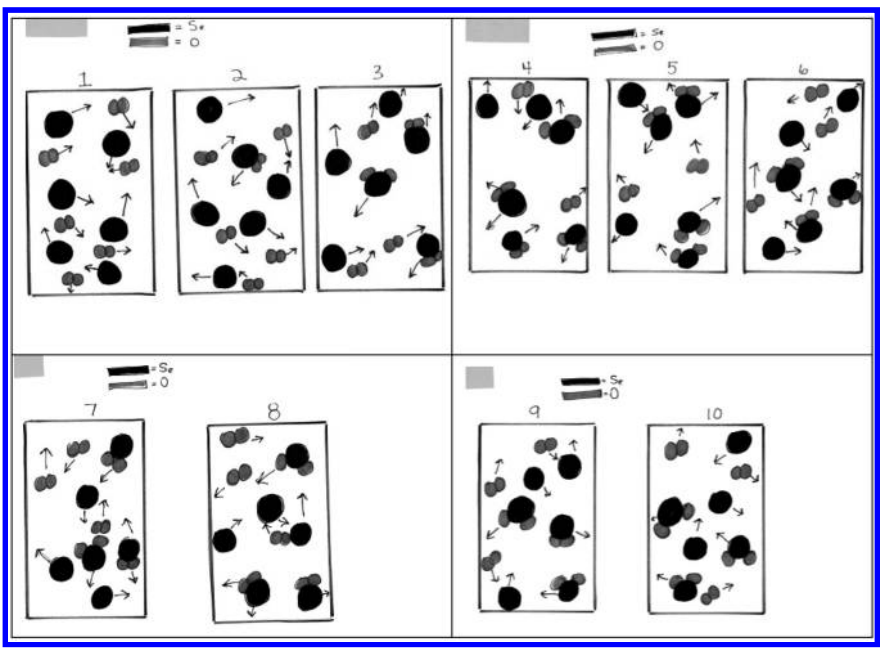

Figure 1. Sample Student Storyboard for Se(g) + O_2(g) $\rightleftharpoons$ SeO_2(g)

Summary

This research project documented how students' mental rotation abilities and content knowledge changed when exposed to one of two methods of modeling an equilibrium process: an animation computer program and a storyboard with paper and pencil. The students significantly gained in equilibrium content knowledge and significantly gained in mental rotation ability, regardless of the method used (storyboards or ChemSense animations). By having students represent the concepts themselves, students are taking an active role in their learning.

This study found that males had a significantly better ability to rotate three-dimensional objects as measured by the Vandenberg test than did the females. Both males and females gained significantly in their mental rotation abilities throughout the course of this project. However, the males' mental rotation ability over the project increased significantly more than that of the females.

Classroom Implications and Further Research

Instructors of general chemistry in college, as well as high school chemistry teachers, should consider including activities designed to help improve the spatial abilities of their students for the following reasons: (a) having good spatial abilities can better equip students to be successful in chemistry (*12*, *13*) and (b) it has been shown that mental rotation ability can be increased in this study and reported by a number of others (e.g. (*28*)). Spatial ability tests, especially mental rotation tests, could be included early in a course to gauge student ability to visualize. In general chemistry and beyond, students need to be able to visualize molecules in three-dimensions, draw them correctly, and answer questions that pertain to their behavior. Exposure to particulate or three-dimensional molecules may be needed throughout courses (*4*). Instructors can use either storyboard or animation assignments to help with equilibrium understanding and mental rotation ability. Each instructor can make the decision about which method would work best after reviewing the logistical situation and resources available at their own institution.

Further research needs to investigate whether storyboards or animations have any effect with other concepts in chemistry. It should be noted that students still have difficulty with equilibrium; therefore, research on how to improve students understanding of physical and chemical equilibria is also needed.

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Chapter 13

How Does the Order of Viewing Two Computer Animations of the Same Oxidation-Reduction Reaction Affect Students' Particulate-Level Explanations?

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This study compares how the order of viewing two different computer animations affects students' particulate-level explanations of an oxidation-reduction reaction. The animations differ primarily in the complexity of the visual images used. The explanations from participants viewing the more simplified animation followed by the more complex animation were compared to those from participants viewing the animations in the opposite order using analysis of covariance, with participants' explanations prior to viewing either animation as the covariate. This comparison showed that those viewing the more complex animation followed by the more simplified animation provided better explanations than those viewing them in the opposite order. These concepts included the absence of ion pairs, the electron transfer process, size changes in the atoms and ions, the source of the blue color in solution, the fact that water was not forcing this reaction to occur, and writing a balanced chemical equation for this reaction. Participants had less difficulty interpreting the more simplified animation, in part because it showed the charges of the atoms and ions, the number of electrons transferred from copper to silver, the 2:1 reacting ratio of silver and copper, the size changes occurring as silver and copper reacted, and the solution becoming darker

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blue every time a copper ion was released into the solution. Comments from participants who believed that showing the more complex animation first and the more simplified animation second was the best way to teach this topic suggested that showing the more complex animation first will get students' attention, and then showing the more simplified animation will explain the chemical reaction and this will lead to improved learning.

Introduction

Research evaluating the effectiveness of computer animations depicting the behavior of atoms, molecules, and ions has shown that these visualization techniques can improve students' particulate-level explanations of chemical phenomena (*1–13*). In his review of the chemical education research involving the use of computer animations, Sanger (*14*) summarized the evidence for the effectiveness of particulate-level computer animations compared to instruction without particulate drawings and to instruction with static particulate drawings, and found that although computer animations can sometimes introduce new misconceptions, these animations appear to be useful in helping students to develop particulate-level understanding of many chemical reactions. This review also suggests that the use of computer animations will be most beneficial to students if the lessons require students to address issues of visualization, motion, or trajectory (*15*). Williamson and José (*16*) has summarized the types of visualization techniques applicable to the chemistry classroom (including computer animations) and Williamson (*17*) used research evidence from chemical education studies on visualization to address possible myths from instructors attempting to incorporate visualization techniques in their chemistry classrooms. Williamson (*18*) also described how chemical education research on students' understanding of the Particulate Nature of Matter has influenced chemistry instruction, standardized examinations, and research conferences.

Several researchers have looked at how the order of presenting two instructional techniques involving computer animations and/or video clips affects students' understanding of chemical reactions. Kelly and Jones (*19*) had students describe the process of solid sodium chloride dissolving in water at the particulate level after viewing a chemical demonstration, and then again after viewing two different particulate-level computer animations of this process. One animation focused on the dynamics and energetics of dissolving, while the other animation focused on structural features. Eleven students viewed the dynamics/energetics animation first and the structural features animation second, and seven students viewed the animations in the opposite order. Kelly and Jones found that students viewing the dynamics/energetics animation changed their conceptions of the dissolving process while students viewing the structural features animation made changes to their self-generated particulate drawings. However, many students had difficulty incorporating the information depicted in the animations in their mental models.

Velázquez-Marcano *et al.* (*8*) asked students to make predictions about the behaviors of gas samples undergoing three different diffusion reactions before and after viewing a video of the chemical demonstration and a computer animation showing the particulate behavior of the gas molecules. Half of the students viewed the videos first and the animations second, while the other half viewed the animations first and the videos second. This study showed that the percentage of students correctly predicting the macroscopic-level behavior of the gas samples improved after viewing the first visualization technique and again after viewing the second visualization technique. The order in which students viewed the two visuals did not appear to affect their abilities to predict the macroscopic behavior of the gas samples. The authors concluded that both the macroscopic depiction of the gas sample from the video and the particulate depiction of the gas molecules from the animation were necessary for students to predict the macroscopic behavior of the gas samples in the three experiments.

In a follow up study, Williamson *et al.* (*13*) compared students' particulate-level explanations of the three diffusion experiments described by Velázquez-Marcano *et al.* (*8*). Half of the students in the newer study viewed the videos first and the animations second, while the other half viewed the animations first and the videos second; both sets of students then viewed the animation and video simultaneously. This study showed that students provided the most correct particulate-level explanations after viewing the particulate animations, they provided the least correct explanations after viewing the macroscopic videos, with an intermediate number of correct explanations after viewing the simultaneous video/animation pairings. This experiment also showed that the order of visuals affected the number of correct particulate-level explanations from students—students were more likely to provide correct explanations if they viewed the macroscopic-level video first and the particulate-level animation second. The authors attribute this preference to the idea that the macroscopic-level videos allow students to become familiar with the experiment and this prepares them for the particulate-level explanation given by the animations.

The goal of this study is to compare participants' particulate-level explanations of an oxidation-reduction reaction involving silver nitrate and copper metal after viewing a chemical demonstration and two animations for this reaction. The two animations depict the same chemical reaction, but at different levels of complexity—the animation created by Michael J. Sanger, referred to as the more simplified animation in this study, uses a static camera angle, does not depict the water molecules, and depicts objects moving on a single plane. The animation created by the VisChem Project (*9*, *20*, *21*), referred to as the more complex animation in this study, uses a changing camera angle, depicts the water molecules, and allows objects to move in front of or behind each other. The labels of *more simplified* and *more complex* were based on the participants' descriptions of the two animations during the interviews (*22*); during the interviews, the Sanger animation was referred to as the *2-D animation* because it was animated in a single two-dimensional plane and the VisChem animation was referred to as the *3-D animation* because it was allowed objects to move in front of or behind each other. Half of the participants in this study viewed the more simplified animation first and the more complex animation second while the

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other half viewed the animations in the opposite order. This study compares the participants' particulate-level explanation of the chemical reaction after viewing both animations.

Theoretical Framework

When discussing chemical reactions, chemists often use three related but distinct representational levels—the macroscopic, particulate, and symbolic levels (*23–26*). The macroscopic representation involves qualitative and quantitative observations of the chemical reaction made using the five senses; the particulate representation involves the behavior of atoms, molecules, and ions in the chemical reaction; and the symbolic representation involves the use symbols (numbers, mathematical formulas, chemical symbols and formulas, balanced equations, etc.) to represent more abstract concepts. This study is focused on students' particulate-level explanations of the oxidation-reduction reaction occurring between copper metal and aqueous silver nitrate.

The effectiveness of instruction using computer animations of chemical processes at the particulate level is based on Mayer's cognitive theory of multimedia learning (*27*), which was adapted from Paivio's dual-coding theory (*28*) and Baddeley's model of working memory (*29*). Mayer's theory assumes that learners possess separate cognitive channels for processing visual (pictorial) and auditory (verbal) information, that learners have limited processing capabilities in each channel, and that learners engage in active learning by attending to relevant information, organizing this information into mental schema, and integrating this new knowledge with pre-existing knowledge.

Mayer's cognitive theory of multimedia learning, which incorporates the information-processing theory of learning (*30–34*) and cognitive load theory (*29*), assumes that learners must attend to external information (ideas, events, or concepts) in their sensory memory and must select this information (based on previous knowledge, interests, prejudices, and beliefs) before they can use it in their working memory. It also assumes that working memory is limited (*35–40*), and learners use their working memory to bring together and incorporate new information from sensory memory and old information stored in long-term memory (*33*, *34*). Schema-activation methods (*33*) assist learners in connecting new material with relevant stored information and can help improve learning. Cueing, which is an example of schema-activation methods, uses instructional methods to activate relevant prior knowledge from long-term memory (*41–44*).

Methods

Sample Size and Selection

The sample included 19 male and 36 female participants enrolled in a second-semester general chemistry course who volunteered to be part of this study.

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These participants were recruited from a single section taught by a chemistry professor with over 15 years of teaching experience at the college level. In order to evaluate the students' conceptual understanding of the oxidation-reduction reaction at the particulate level, each participant was interviewed after receiving lecture instruction on oxidation-reduction reactions and electrochemistry. Each interview took from 40-70 minutes, and the interviews were digitally recorded and transcribed verbatim by the first author. The participants were randomly assigned to one of two groups. Both groups started the interviews by viewing a chemical demonstration involving liquid water, solid silver nitrate, and solid copper metal. The first group ($N = 26$) then viewed a more simplified animation of this chemical reaction followed by a more complex animation of the reaction; the second group ($N = 29$) viewed the more complex animation first and then the more simplified animation.

Interview Script

The questions used for the semi-structured interviews appear in Figure 1. The questions were created by the two researchers based on a list of conceptual and propositional knowledge statements generated by the authors and described in a previous publication (*45*). The content validity of these questions was examined by asking two chemistry professors (each with over ten years of college teaching experience) to determine whether the interview questions address all of the ideas listed in the conceptual and propositional knowledge statements. The questions were adapted based on the professors' comments.

The interviews consisted of three parts. The first part of the interview (questions 1-7) asked participants to explain the particulate-level behavior of the chemicals in the chemical demonstration. In the second part of the interview, participants were asked to watch a particulate-level computer animation of the chemical reaction and explain how their answers in part 1 changed based on viewing the animation. The third part of the interview asked participants to watch another particulate-level computer animation depicting the same chemical reaction and were asked to explain how their answers had changed based on viewing the second animation. The total time to watch each animation was about 30 seconds, and the participants were allowed to replay either animation as many times as they wanted. The audio portion (narration) of both animations was disabled so we could determine how participants interpreted the visual images depicted in these animations. The rationale for showing the animations without the audio portion was that both narrations described the chemical processes occurring in the oxidation-reduction reaction at the particulate level. Therefore, allowing participants to hear the audio tracks would have measured their abilities to hear and repeat the narrated explanations instead of their abilities to interpret and explain the visual images depicted in these animations.

Part 1. Questions asked after the student viewed the demonstration involving aqueous silver nitrate and solid copper metal.

1. How do you know that a chemical reaction is occurring?
2. What substances are present before the reaction? Describe these substances at the particulate level. If you could "see" the atoms and molecules, what would they look like?
3. What are the products of the chemical reaction?
4. What is the function of each substance in the chemical reaction?
5. Where does the chemical reaction occur?
6. Why does the chemical reaction occur?
7. Write a balanced equation for the chemical reaction.

Part 2. Questions asked after the student viewed the first computer animation involving aqueous silver nitrate and solid copper metal.

8. Have any of your answers changed for the appearance of the substances?
9. Have any of your answers changed for the reactants of the chemical reaction?
10. Have any of your answers changed for the products of the chemical reaction?
11. Does the animation change where you think the chemical reaction occurs?
12. Does the animation change why you think the chemical reaction occurs?
13. Write a balanced equation for the chemical reaction.
14. Does the animation help you understand the chemical reaction? If so, how?

Part 3. Questions asked after the student viewed the second computer animation involving aqueous silver nitrate and solid copper metal.

15. Have any of your answers changed for the appearance of the substances?
16. Have any of your answers changed for the reactants of the chemical reaction?
17. Have any of your answers changed for the products of the chemical reaction?
18. Does the animation change where you think the chemical reaction occurs?
19. Does the animation change why you think the chemical reaction occurs?
20. Write a balanced equation for the chemical reaction.
21. Does the animation help you understand the chemical reaction? If so, how?

Figure 1. Interview script used for the semi-structured interviews.

Computer Animations

A still image of the more simplified animation, created by the second author, appears in Figure 2. This animation was created using Macromedia Director, and was designed using principles described by Burke *et al.* (*46*). This animation was designed to be used along with a chemical demonstration and a balanced chemical equation to help students make connections between the three chemical representations (*23–26*) based on student misconceptions of oxidation-reduction reactions identified as part of a classroom assessment. The animation was also carefully designed to accurately depict chemistry content (e.g., silver ions being reduced, copper atoms being oxidized, electrons being transferred from copper atoms to silver ions, the two-to-one reacting ratio of silver ions and copper atoms, etc.); this animation includes an audio narration but water molecules were not depicted so students would focus on relevant information and would not be distracted by irrelevant information (*27*).

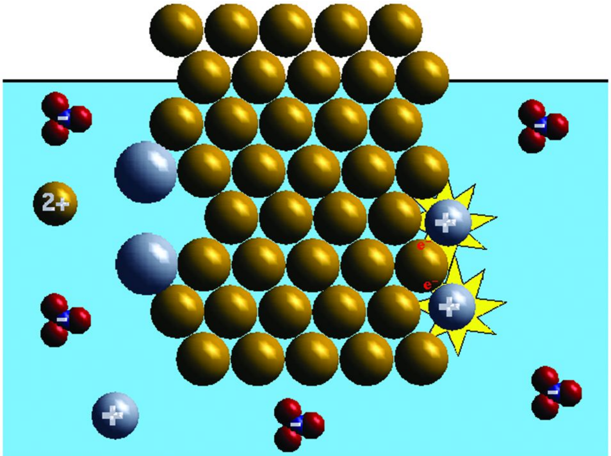

Figure 2. Still image from the more simplified animation. (see color insert)

The more simplified animation begins with several copper-colored circles in an organized 2-D pattern (copper metal) in front of a blue background occupying the bottom part of the screen (water). Floating in the blue background are several silver-colored circles with a '+' on them (silver ions) and an equal number of objects containing one blue circle with a '–' on it surrounded by three red circles (nitrate ions). As the animation progresses, two silver '+' circles approach one of the copper circles. When these three objects collide, two red 'e–' (electrons) appear on the copper circle and move from the copper circle to one of the two silver '+' circles. During this process, the copper circle becomes smaller and now has a '2+' symbol on it and each silver '+' circle becomes larger and loses the '+' symbol (electron transfer). The two silver circles stay with the cluster of copper circles and the copper '2+' circle migrates into the blue background. This process occurs four times throughout the animation; each time, the blue background changes from a lighter to a darker blue color. The blue/red clusters move throughout the blue background and collide with several other objects, but do not change during the animation.

A still image of the more complex animation, designed by Roy Tasker as part of the VisChem project (*11*) and used with his permission, appears in Figure 3. The design principles used to create this animation have been described previously (*21*). This animation begins with several yellow spheres in an organized 3-D pattern (copper metal) in front of a black background. Each of the yellow spheres (copper nucleus and core electrons) is surrounded by a light gray "fuzziness" (valance electrons). The mass of yellow/light gray spheres is surrounded by several red spheres, each with two smaller white spheres attached to them (water molecules). Among the red/white shapes are a few larger gray spheres (silver ions). Occasionally, a cluster containing a blue sphere surrounded by three red

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spheres (nitrate ion) appears among the red/white shapes. As the animation progresses, a gray sphere moves toward the yellow/light gray mass. When they touch, a transparent light gray sphere surrounds the gray sphere (electron transfer) and the gray/light gray sphere remains attached to the yellow/light gray mass. At a different time and spot on the yellow/light gray mass, a yellow sphere loses its light gray outer sphere (electron transfer) and leaves the yellow/light gray mass to move among the red/white shapes. Throughout the animation, two gray spheres become attached to the yellow/light gray mass for every one yellow sphere leaving the mass. The red/white shapes surround the gray and the yellow spheres, pointing their red spheres toward these gray or yellow spheres. The red/white shapes bring the gray spheres to the yellow/light gray mass and pull the yellow spheres away from the yellow/light gray mass. The blue/red shapes move among the red/white shapes, but neither object changes during the animation.

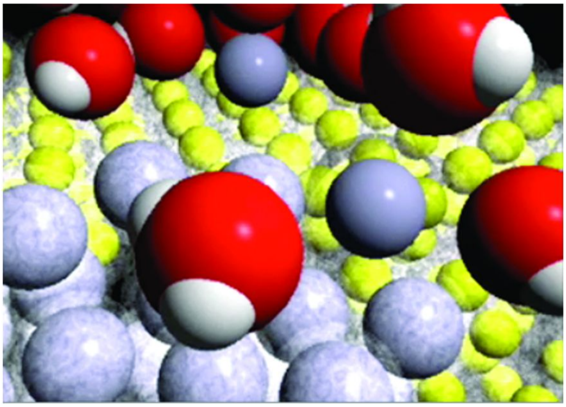

Figure 3. Still image from the more complex animation. Image courtesy of Roy Tasker, University of Western Sydney (20) (see color insert)

Data Analysis

The data analyzed in this study consisted of transcripts of the student interviews. These transcripts were analyzed and categorized into a summary of misconceptions identified from each interview. These summaries were compiled into a list of common student misconceptions. The 21 misconceptions were described in greater detail in another paper (*45*). In the next step of the data analysis, numbers were assigned to the students' concepts based on these misconceptions. Fifteen of the identified misconceptions (*45*) were converted into the nine concepts described in this study. Misconceptions 11 and 14 were based on the comments of a single student, and these misconceptions were not shown by

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any of the other 54 students in the study. Misconception 2 is based on students' misinterpretation of the valence electrons in the copper solid depicted by the more complex animations; however, since the more simplified animation did not depict the valence electrons, no meaningful comparison could be made. Misconceptions 8-10 corresponded to incorrect charges for the ions in solution (i.e., "Ag^{2+}", "NO_3^{2-}", and "Cu^{+}"); these do not refer to actual student conceptions as much as simple errors in propositional knowledge, so they will not be discussed in this paper.

For most of the nine concepts discussed in this study, a score of '0' was given if the student exhibited the misconception or failed to express the correct conception and a score of '1' was given if the student expressed the correct conception. For misconceptions containing multiple ideas, participants were given one point for each idea expressed; these scores will be described in greater detail later in this paper. In addition to the nine concepts, participants were also given a 20-point score for their balanced chemical equation of the oxidation-reduction reaction. Both authors determined concept scores for each student based on each concept; the initial agreement between the two authors' scores was 0.92. Each discrepancy was discussed and a single score was agreed upon by the two authors.

This study is concerned with how participants' explanations of the concepts associated with the oxidation-reduction reaction differ after viewing the two different computer animations depending on whether they saw the more simplified animation first and the more complex animation second (Group SC) or whether they saw the more complex animation first and the more simplified animations second (Group CS). Therefore, participants' concept scores after viewing the second animation were compared using a one-way Analysis of Variance (ANOVA) with the animation order as the independent variable. For any of the misconceptions where concept scores could also be determined for the chemical demonstration interview before viewing any animations, a one-way Analysis of Covariance (ANCOVA) was performed using the animation order as the independent variable and the demonstration concept score as the covariate.

Results

Participants' explanations for the two groups were compared based on the following concepts: Correctly identifying the water sample, correctly identifying the nitrate ions, recognizing the absence of ion pairs in solution, explaining the electron transfer process, recognizing size changes of the silver ion and copper atom, recognizing the source of the blue color in solution, recognizing that water is not the driving force for this reaction, recognizing a 1:1 ratio of silver and nitrate ions, recognizing a 2:1 reacting ratio of silver ions and copper atoms, and writing a balanced equation for the reaction. A summary of the statistical data for these comparisons (including the adjusted least square means and standard errors for the two groups) appears in Table I.

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Table I. Statistical Results for the Comparison of the Two Student Groups.

Concept[a]	*Order Effect*		*Adjusted LS Mean (Standard Error)*	
	F value	*p value*	*SC Group*	*CS Group*
Identifying water*	13.453	0.001	0.538(0.078)	0.931(0.074)
Identifying nitrate*	15.025	0.000	0.462(0.081)	0.897(0.077)
Absence of ion pairs	45.380	0.000	0.382(0.067)	1.002(0.063)
Electron transfer process	85.889	0.000	1.606(0.119)	3.146(0.112)
Atom/ion size changes*	55.433	0.000	0.731(0.124)	2.000(0.117)
Source of blue color in solution	156.588	0.000	-0.017(0.094)	1.636(0.089)
Water is not the driving force (ignoring nitrate)	16.777	0.000	0.596(0.068)	0.983(0.064)
Water is not the driving force (including nitrate)	40.631	0.000	0.389(0.068)	0.996(0.065)
1:1 silver-nitrate ratio	2.891	0.095	0.916(0.038)	1.006(0.036)
2:1 silver-copper ratio	1.756	0.191	0.831(0.061)	0.944(0.058)
Writing a balanced equation	5.206	0.027	17.821(0.478)	19.333(0.452)

[a] NOTE: Concepts with an asterisk have (1,53) degrees of freedom; all other concepts have (1, 52) degrees of freedom. A p value less than 0.05 corresponds to a significant difference between the responses of the two groups of participants.

Identifying the Water Sample

The more complex animation depicted the water sample as water molecules (two white spheres attached to one red sphere), while the more simplified animation show the water sample as the blue background in which the aqueous ions moved. After viewing both animations, 93% of the participants in the CS group correctly identified water as the blue background while only 54% of the SC group correctly identified water as the red/white clusters, $F(1,53) = 13.453$, $p = 0.001$. Most participants in the SC group who incorrectly identified the red/white clusters thought that there were nitrate ions. After viewing the first animation, 62% of the participants in the CS group correctly identified water as the red/white clusters while 92% of the SC group correctly identified water as the blue background. These results suggest that the participants had more difficulty identifying the red/white clusters in the more complex animation as water molecules than they did in identifying the blue background as the water sample in the more simplified animation, regardless of the order in which they viewed the animations.

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Identifying the Nitrate Ions

Both animations depicted the nitrate ions as clusters of one blue atom surrounded by three red atoms; the more simplified animation also labeled each cluster with a minus sign on the blue atom to denote the one-minus charge of the nitrate ion. After viewing both animations, 90% of the CS group correctly identified the nitrate ions while only 46% of the SC group correctly identified them, $F(1,53) = 15.025$, $p < 0.001$. Most CS participants who incorrectly identified the blue/red clusters thought that there were copper ions or the source of the blue color in solution. About half (45%) of CS participants correctly identified the nitrate ions after viewing the first (more complex) animation, while most (92%) of the SC participants correctly identified the nitrate ions after viewing their first (more simplified) animation. These results also suggest that the participants had more difficulty identifying the nitrate ions in the more complex animation than they in the more simplified animation, regardless of the order in which they viewed the animations.

Recognizing the Absence of Ion Pairs in Solution

The misconception that ionic compounds form neutral ion pairs in water has been widely reported (*19*, *45*, *47–53*). Participants were given a score for their demonstration (covariate) and post-animations interviews. After viewing both animations, none (0%) of the participants in the CS group and 62% in the SC group indicated the presence of ion pairs in solution, ($F(1,52) = 45.380$, $p < 0.001$). In comparing the participants' responses after viewing the first and second animation, we found that 14 of the 26 participants in the CS group changed their explanations from having ion pairs to not having ion pairs. On the other hand, 17 out of the 29 participants in the SC group changed their explanations from not having ion pairs to having ion pairs. These results suggest that participants were more likely to see ion pairs in the more complex animation than the more simplified animation, regardless of viewing order.

As an example, one participant from the CS group (CS1) mentioned during the chemical demonstration [CD] interview that the copper(II) nitrate product from the reaction exists as copper and nitrate ions bonded together as ion pairs (score = 0). When describing the more complex animation [CA], he used his belief that ion pairs would exist between copper and nitrate ions to interpret the red/white clusters (water molecules) as nitrate ions (score = 0). When describing the more simplified animation [SA], which did not show water molecules and instead showed isolated copper ions, he stated that the copper ions appeared to be dissociated from the nitrate ions, which contradicted his initial conception (score = 1).

> CS1 [CD]: Copper ions form with the nitrate ions and that is what gives us the blue solution. Copper must drive the silver away from the nitrate in order to bond with it.

> CS1 [CA]: [The red/white clusters are] nitrate, 'cause it is carrying off copper molecules… Silver came in with the reds and whites, so silver

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nitrate came in, and then it goes to the copper. I say they're nitrates. That was a copper going with the nitrate.

CS1 [SA]: It does not look like the nitrates are holding on to them, as opposed to the other video where the nitrates were actually holding on to the copper… No, they [copper and nitrate] are attached. I have to believe they are attached. But, according the diagram they are not.

A participant from the SC group (SC1) stated that silver nitrate would dissociate as ions in water during the chemical demonstration interview. This participant had no trouble identifying the dissociated silver and nitrate ions in the more simplified animation; however, she had more difficulty interpreting the more complex animation, in part because she identified the red/white clusters as nitrate ions. In her explanation, she stated that copper and nitrate ions bonded together, which contradicted her explanations for the first two interviews.

SC1 [CD]: Well, when the water dissolves the silver nitrate, it breaks it apart into separate molecules—ions. A-G, which is silver, has a positive charge and the nitrate would have a negative charge as an ion.

SC1 [SA]: Yeah, silver would be the gray balls with the plus on them 'cause when they separate into ions they are positively charged, and then the nitrates would be the red [and blue] and the negative, but I would not know how to draw them like that…

SC1 [CA]: The red [and white] is the nitrates, silver is silver. It looks like the nitrates are actually attracting the copper away… In some places, it looks like the copper and nitrate combine, which would make sense.

One possible reason for participants seeing ion pairs in the more complex animation is that participants who confused the red/white shapes as nitrate ions saw the gray and yellow spheres (silver and copper ions) surrounded and attached to the red/white shapes, indicating silver-nitrate or copper-nitrate ion pairs. Since the more simplified animation did not depict the water molecules, participants saw only isolated silver or copper(II) ions in solution and did not report seeing ion pairs in this animation.

Explaining the Electron Transfer Process

Each participant earned a four-point score for their explanation of the electron transfer process both before viewing either animation and after viewing both animations. Participants were given one point for mentioning each of the following ideas: Silver ions gain electrons during the reaction, each silver ion gains one electron, copper atoms lose electrons during the reaction, and each copper atom loses two electrons. The adjusted least squares means (corrected for the participants' chemical demonstration scores) were 3.1 out of 4 for the CS group and 1.6 out of 4 for the SC group, $F(1,52) = 85.889$, $p < 0.001$.

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Figure 4 contains a graph of the average participant scores for the electron transfer process for the two groups after viewing the chemical demonstration, the first animation, and then the second animation. The CS group had slight decrease in the electron transfer score after viewing the first (more complex) animation and a large increase after viewing the second (more simplified) animation. The SC group, on the other hand, had a dramatic increase in the electron transfer score after viewing the first (more simplified) animation, but this score dropped after viewing the second (more complex) animation. These results suggest that viewing the more simplified animation helped participants explain the electron transfer process, but viewing the more complex animation was detrimental to the participants' explanations of this process.

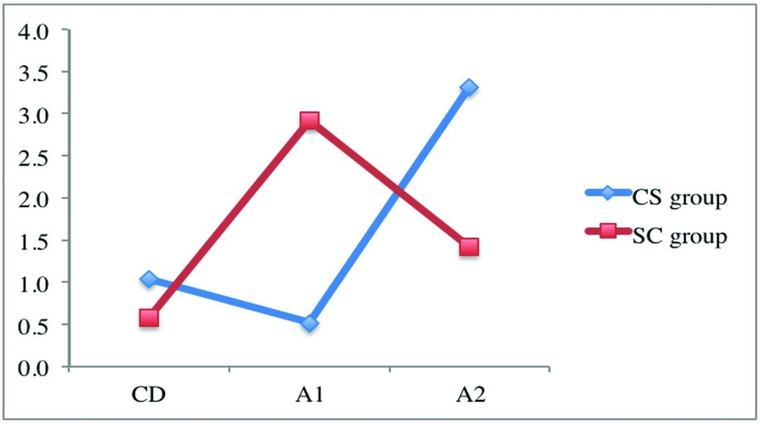

Figure 4. Average electron transfer scores for the CS and SC groups after viewing the chemical demonstration (CD), the first animation (A1), and the second animation (A2).

Quotes from the participants implicate two things depicted by the more simplified animation as being the most helpful in explaining the electron transfer process—explicitly labeling the charges on the atoms/ions and explicitly showing the electrons (depicted as red 'e–' symbols) moving from each copper atom to the silver ions.

> <u>CS2 [SA]</u>: Ah, [the copper ion is] two-plus… So, for every two silvers, one copper comes off. It gives copper a 2 plus charge. Starts out as copper solid, and now copper-II ion in aqueous solution. Losing electrons and being oxidized. Showing two electrons [going] to silver.

> <u>SC2 [SA]</u>: The electrons exchange—two negative.
> *<u>Interviewer</u>: So you see electrons are being exchanged. How do you see that?*
> <u>SC2</u>: The little red e's.
> *<u>Interviewer</u>: Where do the electrons start and where do they end?*

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SC2: From a copper over to a silver. Two electrons come from one copper atom, and one goes to one silver and the other goes to the other silver. Two silvers to one copper.

Participants viewing the more complex animation, however, expressed difficulty in determining the number of electrons being transferred and the charges of the copper or silver atoms being depicted. For example, participant SC3 recognized the addition or loss of the light gray sphere represented electron transfer, but he could not determine how many electrons were transferred or the charges of the objects in the container and did not feel that this animation would help him write a balanced chemical equation for the electron transfer reaction.

Interviewer: So when the silver comes into the surface what else happens to it?
SC3 [CA]: Right now, it does not have its own electron field and when they release it, it develops one. So I guess that means it does now.
Interviewer: So the fuzziness around the surface means it is getting an electron?
SC3: I would assume.
Interviewer: So what happens with the copper, the yellow—is fuzzy and leaves without the fuzzy?
SC3: Well I guess that it is losing an electron, or how ever many it loses. It is not quite clear.
Interviewer: So can you tell charges from this?
SC3: Only if you can stop it to count the number of nitrates that are bonded to each and you know the charge of the nitrates. You can only infer the charge.
Interviewer: Would that help you write the equation? If I had shown you this one first would you have changed your equation much?
SC3: I would not have been able to use this to help change my equation at all. I don't feel I can get a coherent picture of the reaction from this. I have no confidence in any conclusions I drew from that.

Many participants in the SC group provided a complete description of the electron transfer process after viewing the more simplified animation. Unfortunately, they were not always able to apply that answer to the more complex animation and ended up providing less complete explanations for the second (more complex) animation. For example, participant SC1 was able to identify that copper gave up two electrons and that each silver ion gained a single electron in the more simplified animation. When viewing the more complex animation, however, she could see the electron transfer from copper to silver, but didn't mention the charges of the objects in the reaction or the number of electrons transferred from the copper atoms or to the silver ions.

SC1 [SA]: Two silver atoms will only react with one atom of copper, 'cause when two silvers touch, only one copper is released.
Interviewer: What else do you see?

SC1: They are reacting with electrons… You see two silver atoms [sic] react with the copper, and one copper is released that has a plus-two charge. So that must mean that two electrons were donated from the copper, one to each silver. The copper is losing electrons from its valence shell and the silver is gaining electrons in its outer shell.

SC1 [CA]: It is definitely a lot harder to tell the ratios. If I had not already seen the other one I don't think I would know it is two silver to one copper, and here it looks like the nitrates [red/white shapes] are what's pulling copper ions away from… are causing the reaction, I guess.
Interviewer: What about the silver? Is that how you would think it would be depicted?
SC1: Yeah. That is the only time you can see the electrons is when the cloud goes over the silver. The copper… the cloud goes away.
Interviewer: Can you tell where you have something is neutral or charged?
SC1: No, only that the structure of the copper was like that of a solid so you would know the charge is zero.

Recognizing Size Changes for the Silver Ion and Copper Atom

Since none of the participants mentioned changes in size for the silver ions or copper atoms as part of the chemical demonstration interviews, no pre-animation scores were calculated. For the post-animation interviews, participants were given a two point score for size changes—one point for recognizing that silver ions would become larger after gaining electrons and one point for recognizing that copper atoms would become smaller after losing electrons. Participants in the CS group had a mean score of 0.6 out of 2.0 after viewing the more complex animation and a score of 2.0 out of 2.0 after viewing the more simplified animation; participants in the SC group had a mean score of 1.8 out of 2.0 after viewing the more simplified animation and a score of 0.7 out of 2.0 after viewing the more complex animation, $F(1,52) = 55.433$, $p < 0.001$.

Almost all of the participants viewing the more simplified animation correctly identified these size changes, which is not surprising since the animation explicitly depicted the silver ions getting larger and the copper atoms becoming smaller as the electron transfer process occurred. The more complex animation depicted the size changes by adding or removing a transparent light gray sphere from around the yellow or silver spheres representing the copper and silver ions. Unfortunately, many of these participants did not recognize that losing this light gray sphere indicated that the copper atoms became smaller or that gaining this sphere indicated that the silver ions became larger.

It appears that many participants in the SC group were not able to apply their answers regarding the size changes from the more simplified animation to the silver and copper species depicted in the more complex animation.

Interviewer: What happens to the sizes as they react?
SC4 [SA]: Silver getting larger.

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Interviewer: Copper?
SC4: Shrinks—loses its valence electrons.
Interviewer: Why does silver get bigger?
SC4: It gains in the valence shell.

Interviewer: What happens to silver's size?
SC4 [CA]: Same, just fuzzy.
Interviewer: Copper?
SC4: I don't see a size change.

Some participants in the SC group, however, were able to apply their answers regarding the size changes shown in the more simplified animation to the silver ions and copper atoms in the more complex animation.

Interviewer: The gray balls?
SC5 [CA]: The silver that comes out.
Interviewer: What happened to the size as it reacted?
SC5: It should be bigger, but it doesn't look bigger. It kind of stays the same. Looking at the previous [animation] it should be bigger.

Recognizing the Source of the Blue Color in Solution

Participants earned a two-point score for their explanations regarding the source of the blue color in the solution as the oxidation-reduction reaction occurred. Explanations attributing the color to the free (or hydrated) copper(II) ion earned two points, explanations suggesting that copper(II) nitrate or the combination of copper and nitrate ions caused the blue color earned one point, and all other explanations earned zero points. Participants in the CS group had mean scores for the chemical demonstration, the more complex animation, and the more simplified animation of 0.7, 0.7, and 1.6 (out of 2.0), respectively. Participants in the SC group had mean scores for the chemical demonstration, the more simplified animation, and the more complex animation of 1.1, 1.7, and 0.0 (out of 2.0), respectively ($F(1,52) = 156.588$, $p < 0.001$).

Most participants viewing the more simplified animation recognized that the free copper ion was responsible for the blue color in solution. Comments from the participants suggest that the animated color changes of the blue background and animating the copper ions and nitrates as being dissociated helped the participants to recognize copper ions as the source of the blue color. Participants viewing the more complex animation, especially those confusing the red/white shapes as nitrate ions, often suggested that it was a combination of copper and nitrates that made the solution blue.

The following quotes from participant CS3 showed that while explaining the chemical demonstration, he was unsure of whether copper and nitrate ions would form ion pairs in solution. In explaining the source of the blue color after viewing the more complex animation, he was unsure as to whether the blue color came from the copper ions or copper(II) nitrate; however, the more simplified animation appeared to help him decide that the free copper ions caused the blue color.

CS3 [CD]: I know that the silver nitrate dissociates, which enable the copper to displace the silver and silver is able to become a solid. What I am not sure of is how copper is able to get free to bond to nitrate.

CS3 [CA]: What I don't know is if it is just the copper atoms going into solution that causes the color, or the copper atoms going into solution and reacting with nitrate to form copper nitrate that is causing the color change.

CS3 [SA]: I am not sure [what caused the blue color]. Either the copper solution or copper nitrate solution. I see it getting darker. I see the nitrate is not doing much but bouncing off copper solid, and copper ions also. But every time two silvers crash into the copper solid, causes a copper ion to be released the blue gets a shade darker. So, at this point I would say the blue in the reaction is caused by copper ions in solution rather than copper nitrate in solution.

Some of the participants viewing the more complex animation also attributed the blue color in solution to the blue nitrogen atom in the nitrate ion. It is interesting that none of the participants attributed the blue color in solution to the nitrogen atom in the nitrate ion for the more simplified animation.

Interviewer: Does this animation help you figure out what is causing the blue color?
SC6 [CA]: No, because you don't get any background changes, you just see the molecules reacting, just the individual pieces. You don't see anything about the medium or the visual part, like our perspective what we are seeing in real life.
Interviewer: Maybe we can find a blue… (un-pausing the animation)
SC6: *(pointing to a blue/red shape)* It does look like the same blue that the water turned.
Interviewer: So you think the blue is depicting the color of the liquid?
SC6: Possibly.

Recognizing that Water Is Not the Driving Force for the Reaction

The creators of the more complex animation reported that student explanations of their animation indicated some students believed the water molecules were causing the reaction to occur by pushing silver ions toward the copper surface and pulling copper ions away (*9*, *21*). Participants were given a score for their demonstration (covariate) and post-animations interviews. Before viewing either animation, 7% of participants in the CS group and 19% in the SC group made comments suggesting that water was actively driving the reaction. After viewing both animations, none (0%) of the participants in the CS group and 42% in the SC group indicated that water was driving this reaction to occur, $F(1,52) = 16.777$, $p < 0.001$. If we include the number of participants mistaking the red/white shapes

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as nitrate ions who suggested that the nitrate ions were driving the reaction, the percentages of incorrect responses change to 0% for the CS group and 62% for the SC group, $F(1,52) = 40.631$, $p < 0.001$.

In comparing the participants' responses after viewing the first and second animations, no participants (0%) in the SC group suggested that water was driving this reaction after viewing the first (more simplified) animation, and that 38%/66% of the participants in the CS group suggested that water molecules/"red/white shapes" were driving this reaction after viewing the first (more complex) animation, respectively. These results suggest that participants were more likely to believe that the red/white shapes in the more complex animation were driving the reaction compared to the images shown in the more simplified animation, regardless of the order of viewing the animations.

Interviewer: What is the driving force—why this reaction occurs?
CS4 [CA]: The water.
Interviewer: What is the water doing?
CS4: It is pushing the silver into the copper.
Interviewer: Is it also helping with the copper when it leaves?
CS4: Yeah, it is like pulling the copper.

For some participants in the SC group, their correct interpretations of the first animation did not appear to affect their interpretations of the second animation. For example, participant SC2 stated that the nitrates in the more simplified animation were acting as spectators and were not involved in the reaction. However, when viewing the more complex animation, he misidentified the red/white shapes as nitrate ions and talked about how they were causing the reaction to occur by directing the silver ions to the copper surface and directing the copper ions away from the surface.

SC2 [CA]: I see the coppers being released, but… See, the nitrates holds—takes on the silver that is being released. I mean not the silver, but the copper.
Interviewer: From the first animation it looked like the nitrates were not doing anything, right?
SC2: M'hm.
Interviewer: What do you think they are doing here?
SC2: They are directing the silver over to the copper for it to react, and then once the reaction releases the copper, they are directed away from the rest of it.
Interviewer: So they are actually more active in the reaction, right?
SC2: Yeah.

However, other participants in the SC group were able to apply their correct interpretations of the first animation to their interpretations of the second animation. After viewing the more simplified animation, participant SC6 stated that water was needed for the reaction in order to get ions that are part of the reaction. After viewing the more complex animation, she was troubled by the fact that the red/white shapes appear to be more active in the reaction and expressed that she didn't believe that water is forcing the reaction to occur.

> Interviewer: *What is water's role in this reaction—just letting it happening or causing it?*
> SC6 [CA]: It is a spectator. But it looks like it is grabbing. The other one looked like the silver came in and reacted and the copper left. This one [more complex animation] looks like silver is coming in and reacting with copper, and here comes water molecules and grabs a copper. I still don't think it is doing anything.

Recognizing a 1:1 Ratio of Silver and Nitrate Ions

Although some participants explicitly mentioned a 1:1 silver-nitrate ratio in their interviews, many more did not talk about these ratios. In addition, these interview comments seemed to focus on the images depicted in the second animation instead of the participants' personal views of the chemical reaction (similar to the examples shown in many of the quotes described in the previous sections). However, we were able to determine whether the participants believed that silver nitrate existed as a 1:1 ratio of ions by looking at the chemical formula of silver nitrate in their self-generated chemical equations for the chemical demonstration interviews and for the interviews after viewing both animations.

About 55% of participants in the CS group and 77% of participants in the SC group wrote a chemical formula for silver nitrate showing a 1:1 ratio in the interviews about the chemical demonstration. After viewing both animations, 100% of participants in the CS group and 93% of participants in the SC group wrote silver nitrate with a 1:1 ratio of ions ($F(1,52) = 2.891$, $p = 0.095$). These results suggest that both groups of participants learned this concept rather well, regardless of the order in which they viewed the two animations.

Recognizing a 2:1 Reacting Ratio of Silver Ions and Copper Ions

Similar to the concept regarding the 1:1 silver-nitrate ratio, we found that most participants' comments during the interviews focused on the images depicted in the second animation instead of their personal views of the reaction, so we also used the participant-generated balanced equations to determine whether they believed that silver ions and copper atoms reacted in a 2:1 ratio.

About 14% of participants in the CS group and 23% of participants in the SC group wrote a balanced chemical equation showing a 2:1 ratio for silver nitrate and copper metal in their interviews about the chemical demonstration. After viewing both animations, 93% of participants in the CS group and 84% of participants in the SC group wrote balanced chemical equations with a 2:1 ratio of silver nitrate and copper metal ($F(1,52) = 1.756$, $p = 0.191$). These results also suggest that both groups of participants learned this concept rather well, regardless of the order in which they viewed the two animations.

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Writing a Balanced Equation for the Reaction

As part of the interviews, participants were asked to write a balanced chemical equation for the reaction. Each participant was given a 20-point score for their balanced equation based on the chemicals present in the equation (formulas, charges, states of matter), stoichiometric ratios, and atom and charge balance. From the chemical demonstration interviews, the CS group had an average score of 14.5 out of 20 and the SC group had an average score of 15.6 out of 20; these values were used as a covariate for the ANCOVA calculations. The adjusted least squares means (corrected for the participants' chemical demonstration scores) after viewing both animations were 19.3 out of 20 for the CS group and 17.8 out of 20 for the SC group, $F(1,52) = 5.206$, $p = 0.027$.

Figure 5 contains a graph of the average participant scores based on their balanced chemical equations for the two groups after viewing the chemical demonstration, after viewing the first animation, and then after viewing the second animation. There was little to no change in the average participant scores after viewing the more complex animation (from CD to A1 for the CS group and from A1 to A2 for the SC group); however, there was a large increase in the average participant scores after viewing the more simplified animation (from A1 to A2 for the CS group and from CD to A1 for the SC group). However, this increase was larger for the CS group than the SC group ($t_{41} = 2.151$, $p = 0.038$), and this appears to be the cause of the difference between the average scores for the two groups after viewing both animations.

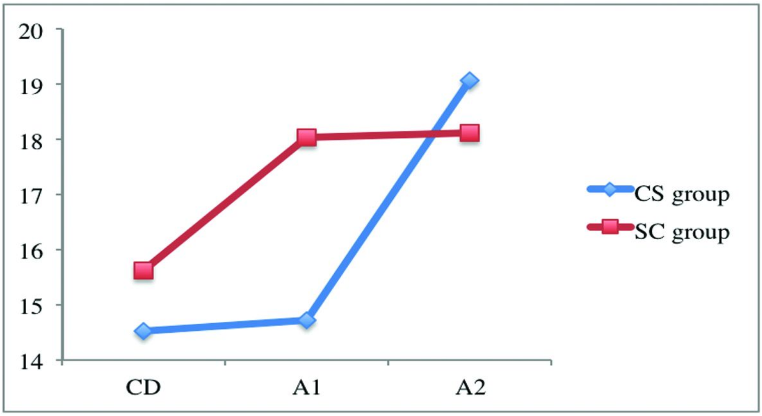

Figure 5. Average balanced equation scores for the CS and SC groups after viewing the chemical demonstration (CD), the first animation (A1), and the second animation (A2).

Quotes from the participants showed that the more simplified animation seemed to help them write a balanced equation by showing the atom and ion charges, by explicitly showing the number and direction of electron transfer, and by more obviously showing the 2:1 reacting ratio for silver nitrate and copper. The more complex animation, however, was not as helpful because it did not show

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the charges or the number of electrons transferred. As an example, participant CS5 stated that the more complex animation did not change his balanced equation (based on the chemical demonstration) because he did not know the charges of the silver or copper ions. Since the more simplified animation had the atom and ion charges labeled, this helped him write the correct formula for copper(II) nitrate and to write a balanced equation with a 2:1 stoichiometric ratio for the silver and copper species.

> *Interviewer: Balanced equation? Does this animation make you change your answer?*
> CS5 [CA]: I don't believe so. The only issue that remains is the charges. If I knew the charges of silver and copper, I would know charges of nitrate and that would change my subscripts.
>
> *Interviewer: Does that [animation] help?*
> CS5 [SA]: Very helpful, since I did not have charge memorized. So, in copper nitrate there would be one copper for two nitrate.
> *Interviewer: Would this change your balanced equation?*
> CS5: Indeed it would. *(rewrites equation)*
> *Interviewer: What is the '2' in front of A-G and A-G-N-O-3?*
> CS5: Two moles.
> *Interviewer: Do you see that in the animation?*
> CS5: Yes, that seems to be represented. The gray balls—silver—need… two of them need to smack into the same copper molecule [sic] to get the copper off the solid.

The more simplified animation helped participant SC7 recognize that copper ions have a plus-two charge and that there was a 2:1 reacting ratio for silver ions and the copper atoms. However, she felt that the more complex animation was not helpful and would have led to an incorrect balanced equation because she would not have seen the 2:1 ratio in the copper(II) nitrate product.

> *Interviewer: Do you think this [more simplified animation] helps you write the balanced equation?*
> SC7 [SA]: We will have 2 of these for every one copper. Copper has a two-plus charge. C-U-N-O-3-2.
> *Interviewer: Why did you put '2' in front of nitrate and silver?*
> SC7: Two silvers for every one copper.
> *Interviewer: That came from [the] animation or balancing?*
> SC7: We started from animation.
> *Interviewer: What did the animation help you with?*
> SC7: Well, when copper comes off, it is two-plus.
> *Interviewer: So that helped you change the formula for copper nitrate?*
> SC7: Right, and then we could balance the rest of that.
> *Interviewer: Does this [more complex] animation change your balanced equation?*
> SC7 [SA]: No.

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<u>Interviewer</u>: *Does it confirm the formula?*
<u>SC7</u>: I think it hurts 'cause I would just do the same formula and not take this animation into consideration. If we had watched this [animation] first, we would not have gotten two nitrates for every one copper.

In any event, after viewing both animations the average participant scores for both groups were above 18 out 20. This result suggests that viewing the chemical demonstration and the two animations helped the participants understand this reaction well enough to write appropriate balanced chemical equations for the reaction, regardless of animation order, although the CS group slightly outperformed the SC group in writing accurate balanced equations.

Participants' Opinions Regarding Animation Order

After viewing both animations, the participants were asked whether an instructor teaching about oxidation-reduction reactions should use none, one, or both of these animations. For the participants who indicated that both animations should be shown, they were asked in which order the animations should be shown. For the participants in the CS group, six (23%) suggested showing only the more simplified animation, sixteen (62%) suggested showing the more simplified animation followed by the more complex animation, and four (15%) suggested showing the more complex animation followed by the more simplified animation. For the participants in the SC group, these numbers were eight (28%), ten (34%), and eleven (38%), respectively. None of the participants in either group suggested showing only the more complex animation. Based on a chi-square test of homogeneity, these distributions for the two groups are not statistically different ($\chi^2(2) = 4.788$, $p = 0.912$).

For the participants suggesting that the instructor should only show the more simplified animation, most of them stated that the more simplified animation was easier to understand and that the more complex animation was confusing.

<u>Interviewer</u>: *Do you think we should show both [animations]?*
<u>SC8</u>: I don't know if both are necessary. This one [more simplified animation] is a lot easier to understand… The other one is more realistic, but I am never going to picture it the way the [more complex] one is. It is too complicated. It is more confusing.

Most of the participants suggesting that the instructor should show the more simplified animation first followed by the more complex animation based their answer on the belief that students would be able to follow and understand the more simplified animation, and that this would help them make sense of the more complex animation.

<u>Interviewer</u>: *Does [animation] order matter?*
<u>CS6</u>: I think this animation [more simplified] is a lot more clear. If you want to start off general and provoke questions from the class, I would keep the order. 'Cause this one is much more specific, it could bring up topics such as size of ions versus non-ions, as well as color change, ratios.
<u>Interviewer</u>: *You think [more simplified] then [more complex]?*
<u>CS6</u>: Yeah, 'cause I think this one explains things better. The first one, there is a lot of things you can miss.

<u>Interviewer</u>: *Should we show one animation, no animations, or both?*
<u>SC9</u>: I would show both. Show [the more simplified one] first.
<u>Interviewer</u>: *Why?*
<u>SC9</u>: That way they [students] know what the charges are before they see the [more complex] one.
<u>Interviewer</u>: *What would happen if you showed the [more complex one] first?*
<u>SC9</u>: I would be like, 'Huh?' The first one shows basically what is happening. The second shows what it would look like. The charges and then the movement.

For the participants suggesting that the instructor should show the more complex animation first followed by the more simplified animation, there were two types of answers. The first idea (mentioned by four participants) was that the more complex animation will capture students' attention and then the more simplified animation will actually explain the reaction. The second idea (mentioned by seven participants) was the more complex animation will confuse or disequilibrate the students, and then the more complex animation will alleviate this confusion.

<u>Interviewer</u>: *If you were going to teach this in a class, would you show just one of them, or both of them, or none of them?*
<u>SC5</u>: Actually, I would show both. …but if I would, [I] probably show the second one that you have shown us before the other one, so you could say 'Ooh, this is how it all looks' and you could see the atoms all moving around and the second one… if you showed it after this fancy one, then this is actually what is happening and these are the charges reacting. Just a little more simplistic. The [more complex] one would get their attention and get them interested and get them wondering, and then the [more simplified] one would break it down.

<u>Interviewer</u>: *Do you think we should show both [animations]?*
<u>CS7</u>: Yes.
<u>Interviewer</u>: *Do you think order matters?*
<u>CS7</u>: Show [the more simplified] last. This is going to seal the deal. If they don't get [the more complex one], they will get this. You don't want to show something that majority of people will get first, and then show them something that will kind of confuse them.

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Discussion

The results of this study showed that the order of viewing the two animations significantly affected the participants' particulate-level explanations of the oxidation-reduction reaction occurring between silver nitrate and copper metal. Specifically, participants viewing the more complex animation created as part of the VisChem Project (*9*, *20*, *21*) first and the more simplified animation created by Michael J. Sanger (*14*, *45*) second (group CS) provided more correct explanations of this reaction than students viewing the more simplified animation first and the more complex animation second (group SC). These improved explanations included accurately identifying water and nitrate ions, recognizing the absence of ion pairs in solution, explaining the electron transfer process, recognizing size changes of the silver ion and copper atom, recognizing the source of the blue color in solution, recognizing that water is not the driving force for this reaction, and writing a balanced equation for the reaction.

Comments from some of the participants showed that their explanations were focused on the last animation viewed and not on the chemical phenomena being depicted in the animations. Tasker and Dalton (*21*) noted that students viewing their animations could transfer ideas learned from their animations to similar situations, but not to new topics, which they interpreted as a lack of these key features being internalized by the learners. In this study, our participants had limited success in internalizing the ideas learned from either animation, focusing on the images depicted by a particular animation instead of applying them to their mental models of the chemical system, and that they had difficulty applying concepts depicted in one animation to the images depicted in the other.

Based on participants' comments, the more simplified animation was easier for many of them to interpret than the more complex animation. Several of the participants stated that the more simplified animation was easier to understand because it did not show so many water molecules. Since most of the concepts tested in this study (which were based on misconceptions identified from the participants' explanations of the oxidation-reduction reaction depicted in the animations) could be adequately explained without invoking the role of the water molecules, their depiction in the more complex animation may have distracted participants' attention away from the more relevant information, increasing the extraneous cognitive load of the instructional lesson (*9*, *37*, *38*). The negative effect on increasing extraneous load is consistent with Mayer's coherence principle (*27*), which states that learning is improved when extraneous material is excluded rather than included, and is also consistent with cognitive load theory (*29*, *35–40*). Comments from the participants' interviews also showed that the more simplified animation was easier to interpret because it showed the charges of the atoms and ions, showed that each copper atom lost two electrons and that each silver ion gained one electron, more clearly showed the 2:1 reacting ratio of the silver ions and copper atoms, showed the size changes occurring as the silver ions and copper atoms reacted, and showed that the solution became darker blue every time a copper ion was released into the solution. Lee *et al.* (*39*) showed that providing iconic information in addition to symbolic information in the visuals of an animation improved lower-level comprehension and higher-level learning

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compared to lessons providing only the symbolic information due to a decrease in the extraneous cognitive load of those instructional lessons (*9*, *37*, *38*). The more simplified animation in this study provided additional, iconic, information in the form of atom/ion size changes, depicted ion charges, and background color changes in addition to the symbolic information presented by the more complex animation (ion movement, electron transfer, stoichiometric ratios, etc.). Based on participant comments, inclusion of this information in iconic form improved participants' explanations of the more simplified animation compared to the more complex animation.

However, there were comments from participants stating that their explanations of the second animation were informed by their interpretation of the animation seen in the previous interview. Therefore, it is reasonable to expect that there was an order effect for some of the concepts discussed in this paper, especially concepts tied to writing the balanced chemical equation that encouraged participants to think about the chemical reaction more broadly instead of focusing on the images depicted by a single animation. About 27% of the participants in this study believed that showing the more complex animation first and the more simplified animation second would be the best way to use these animations when teaching about oxidation-reduction reactions. The reason these participants favored this order is that showing the more complex animation first will either entertain students or confuse them and let them know that they don't understand what is happening in the chemical reaction. Once the students' attention has been piqued (by entertainment or confusion), they are now primed and ready to learn, and showing them the more simplified animation will more clearly explain what is happening in the chemical reaction and will lead to improved learning. These participant explanations imply that the more complex animation can cue students to activate relevant prior knowledge from their long-term memory (*41–44*), which assists subsequent learning from the more simplified animation. This order of showing the more complex animation followed by a more simplified animation of the same reaction is also supported by the *VisChem Learning Design* (*9*, *21*), one of the exemplary ICT-based learning designs selected by Australian university educators to foster the use of innovative teaching and learning approaches in Australian universities. In this lesson design, students are first shown a chemical demonstration, then shown a complex animation without narration, followed by simpler chunks of the animation (to reduce the cognitive load on working memory) that are narrated.

Possible Limitations of This Study

Whenever the designer of an instructional tool performs research comparing this tool to one designed and created by others, there is the potential for personal bias, and recognizing this potential for bias is the first step in minimizing it. As chemical education researchers, we have made every attempt to ensure that our comparisons of these two animations were based on actual participant comments.

One of the major limitations of this study was that both animations were used without their supporting narration. Mayer (*25*) asserts that students will learn better if provided information using both the visual and verbal channels (animation and narration), and both Sanger (*3–5*, *10*) and Tasker (*9*, *21*) have demonstrated that narrated versions of their animations can positively affect students' conceptual understanding of chemical processes at the particulate level. Therefore, these results could be very different if the participants had viewed these animations with narration. Future research should be performed using these animations with narration to see if the results are different.

Another limitation identified in this study was that some participants' explanations after viewing the second animation seemed to focus on interpreting that particular animation instead of explaining their mental model of the chemical reaction. Therefore, it might be useful to repeat this study in which the participants are asked to focus their explanations on the actual reaction and not on interpreting the specific animation being watched. This study might be able to determine whether the superiority of the explanations from the CS group over the SC group came from the fact that the participants were focusing their explanations on interpreting the last animation they were watching, or whether viewing the more complex animation first and the more simplified animation second actually leads to improved conceptual understanding of the chemical reaction shown in these animations.

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Chapter 14

The Future of Computer Simulations Designed for Classroom Instruction

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Two pathways for the future of educational design in computer simulation technology are proposed in this chapter. Design in this context refers to both the design of the simulation and its interface and the design of pedagogic activities that integrate this technology. In this chapter, the author will: 1) present a classification scheme for digital technologies in education and determine where computer simulations fall within this scheme, 2) offer comparisons of different types of computer simulations in chemistry education and their external representations, 3) put forward new design directions on the use of non-standard external representations, such as analogic representations and, 4) draw upon three empirical studies to outline how such analogic computer simulations can be used productively in the chemistry classroom with a non-traditional pedagogic design. The first two studies investigate a simulatation with a dynamic analogy, and a third study investigates how a technology-enhanced approach to instruction contributes to student understanding of chemistry in the classroom. Research on this simulation and the instructional approach might be of interest to educators and developers who are exploring the future of design for computer simulations within classroom environments.

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There are an array of digital technologies available to educators and ascertaining the function of computer simulations in this array is important to their study. The first part of this chapter seeks to situate where computer simulations might fall within this array. The second part draws upon three empirical studies with chemistry students in classroom environments to discuss salient design features of computer simulations and the activities that are possible with them.

Part One: Situating Computer Simulations within Educational Technology

Introduction

An array of digital technologies are currently available for chemistry educators to construct complex molecular models (HyperChem, RasMol), display unobservable processes (PhET, NetLogo), search large databases of chemical structures (ChemSpider, Protein Data Bank), represent the results of simulated chemistry lab experiments (the Virtual Lab; irYdium), input data or information and rapidly represent it (e.g. graphing programs), and communicate with peers and experts (e.g. online chemistry and science communities, discussion groups, and e-bulletin boards), to name a few. To help us consider computer simulations within this array, Jonassen and Carr's (*1*) well-known mindtools scheme portrays digital technologies for education as falling into six main categories of affordances for learning. These six categories include: semantic organization tools (databases and semantic organization tools), dynamic modeling tools (expert systems), conferencing environments, knowledge construction environments (hypermedia, web publishing), information interpretation tools (interactive visualizations and search engines), and video (visualization). Over the years, the mindtools scheme has been especially useful for science educators who have based their primary selection of digital technologies on the cognitive and social affordances of each; however, the distinction among simulations and between simulations and animations has not yet been established. As well, some of Jonassen's categories have recently merged with others, making cross-categorical affordances possible (e.g. expert systems that afford visualization and search capacities). A reworked example of a mindtools classification scheme might therefore bring together modeling tools with knowledge construction environments and information interpretation tools in a larger category of "dynamic representations" that present these functional capacities within one application or site. A merger of this sort would reduce Jonassen's top-level categories to four from six. Furthermore, it may also assist in portraying the functions of modeling, knowledge construction, and information interpretation as inter-related and help to distinguish among their sub-categories, such as computer simulations, animations, and other interactive computer tools.

A Classification Scheme for Educational Technology Including Computer Simulations

To begin to situate computer simulations underneath "dynamic representations" and to better delineate them from animations or other information interpretation tools and knowledge construction environments (not listed), several sub-categories of simulations are suggested in Figure 1. This figure does not portray all of the possible categories of educational technologies for chemistry education as per Jonassen's mindtools; it focuses on the dynamic representations strand and only simulations. For the purposes of this chapter, a simulation will be referred to as a program that allows the user to interact with (i) a digital representation of a model of the natural or physical world, or (ii) a theoretical system, and then change it based on inputs by the user. Instructional or educational simulations are those types of simulations that are designed purposefully to function within a learning environment (*2*, *3*). The learning environment in science may have multiple learning goals, such as: learning about mechanistic procedures (*4*), processes such as generating testable relationships about error in chemistry titration experiments (*5*), or conceptual differences between heat and temperature in thermodynamics (*6*). The sub-categories of computer simulations in Figure 1 are based upon what is primarily being simulated in the digital technology. For example, in chemistry education, the four sub-categories of computer simulations are: system models, dynamic emergent systems or microworlds, chemistry information derived from lab results (lab information), and nanoscale or molecular level processes. While clearly not all simulations in chemistry education can be captured by this designation, preliminary surveys of simulations suggest that a number of them can be grouped in one (or more) of these sub-categories. Figure 1 suggests the sub-categories of simulations below.

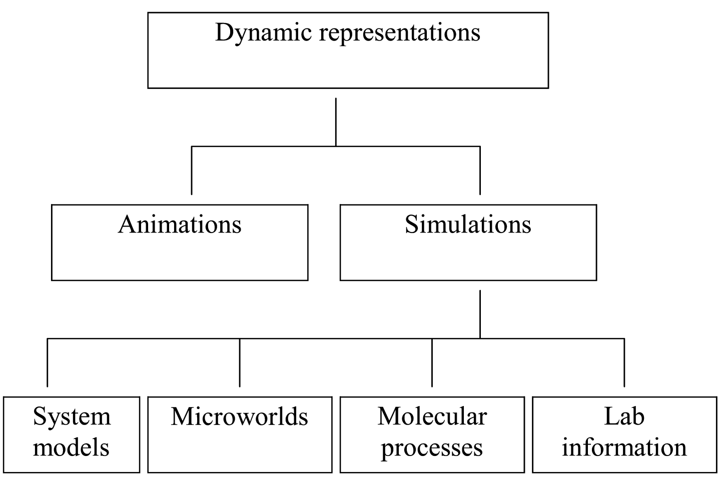

Figure 1. Several sub-categories of computer simulations for learning chemistry.

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Comparisons among Computer Simulations in Chemistry Education

The sub-categories of simulations suggested in Figure 1 are not mutually exclusive; however, there are subtle differences suggested among the four types of simulations in chemistry education: system models, microworlds, lab information, and molecular processes. For those simulations that are primarily system models, for example, the learner can not only manipulate variables of the system being modeled, but might be able to also add, delete, or modify the variables and parameters underlying the model or the relations between them. These system models simulations allow the user to see inside "the glass box" and build a runnable model rather than manipulate an existing one, such as the NetLogo simulations (*13*). In some sense, users can manipulate the program that drives the simulation.

Microworlds, on the other hand, are highly complex simulations that enable users to explore a particular problem area by inventing their own activities and experiments in a realistic setting. Although learners may have extra tools such as expert feedback and databases at their disposal, the setting intentionally bears close resemblance to reality in order to encourage a more natural learning process (*7*). Consequently, learners engage in a self-regulated exploration process by which the major principles of the microworld remain to be discovered (*8*) until instructional interventions interrupt this process of discovery learning. Microworlds allow the user greater control over the experimental design and set up. For example, microworlds of lab experiments allow the user to "hand pick" the glassware for the lab experiment. Second Life, a 3-D virtual environment, contains microworlds for chemistry lab experiments and teaching VSEPR theory.

Lab information refers to simulations that are based on data from lab or other experiments. Chemland's calorimetry simulation (*9*) would be an example of this type of simulation as it contains a schematic of a calorimeter that can be manipulated in terms of the amount of water and the compounds selected to be in it. A graph of the change in temperature in the calorimeter is generated when the user presses start. The graph is generated based on information from laboratory research done by others. This type of simulation is distinguishable from microworlds in that it does not replicate a lab environment or even a calorimeter but rather depicts relationships between two or three variables at most. It is also distinguishable from system models in that minute changes to the system are generally not depicted.

Several computer simulations for chemistry education primarily focus on displaying and manipulating chemical interactions at the atomic and sub-atomic scale. There may be a choice of molecular models to display and the capacity to rotate them. Being simulations, the digital environment is modifiable with input from the user. Examples of simulations that are primarily about molecular processes include several of the free, open source Molecular Workbench applets from the Concord Consortium, such as their states of matter and equilibrium applet. A second example are some of the freely available simulations from PhET, such as the Salts and Solubility and Greenhouse Effect simulations (e.g. see PhET chapter in this book). Ultimately, it is recognized that not all simulations can be neatly captured by a schema such as the one suggested in Figure 1, but the

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process of identifying types of simulations and where they are situated among the array of educational technologies available begins to delineate their uses for chemistry education.

In continuing with the comparisons in Figure 1, the computer simulations do have several features in common across all sub-categories, such as their external representations. Similarities among these simulations permits an examination of their contributions as a whole and also helps to identify possible design options that are not common among them. External representations that tend to be designed include: text-based symbols (e.g. chemical reactions, periodic table), graphical representations (e.g. depicting concentration changes over time), molecular animations (e.g. 3-D balls or related models), animated lab environments, and videos of lab-based experiments. The use of these simulations with multiple external representations (MERs) have been associated with gains in student understanding in chemistry (*10*, *11*). Since 2000 (*12*, *13*), MERs have arguably become standardized in the design of computer simulations for chemistry education. It has been hypothesized that MERs serve to provide chemistry students with additional information about the phenomenon in question, constraints to complex abstractions to help simplify the model, referential connections to the domain under study, visualizations of the dynamic and interactive dimensions of a model, and transformations between 2D and 3D images (*14–17*). Finally, comparisons of the different types of simulations and their MERs, for example, can potentially also assist in putting forward new design directions for computer simulation design, such as the analogic representation discussed in the next part of this chapter.

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Part Two: A New Design Direction for Computer Simulations-the Analogical Representation

Introduction

Recent research in science education puts forward a non-standard external representation for consideration, an analogic representation, in the design of simulation interfaces. The use of analogies to teach science and chemistry in the classroom has had a relatively long history (*18–24*). Common analogies that have been used to teach chemical equilibrium in the classroom, for example, include: the Dancing Couples analogy, Throwing Apples Analogy, the Balance Beam, The Fish Aquarium Analogy, and The Juggler Analogy (*25*). The use of analogy as a representational device in software design, however, has been relatively under-explored compared to other more standard MERs.

This next section brings together the results of two existing research studies on analogies in the design of educational simulations that suggest how animating them supports student understanding in chemistry. The first study used comparative quantitative measures to assess student achievement in chemistry and hypothesized how animating a balance beam as an analogy to chemical equilibrium helped high school chemistry students understand the topic. The second study employed quasi-experimental research to suggest how

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such animated analogies appear to mitigate robust alternative conceptions about chemical equilibrium.

An analogy can be considered at its most fundamental level as a comparison of elements or relations (*26*). Gentner and Gentner (*18*) suggest that such comparisons are particularly beneficial for students' cognitive development because analogies can help students build on their prior knowledge. This building of knowledge can be accomplished by constructing similarities between what is already known and what is unknown or unfamiliar in science (*27*, *39*). To optimize their instructional effectiveness, however, accurate mapping of similarities and differences between the analogy and the target system must occur (*19*, *20*).

In traditional classrooms, analogies are often presented verbally by teachers or in the form of text and images. To further enhance students' visual perception of a phenomenon, however, some of the unobservable relationships that comprise the phenomenon may be depicted via analogies that are made dynamic, or runnable. "Dynamic analogies" have the potential to enhance student understanding of important relationships in science by capturing and depicting the relationships "in action" through a more accessible and familiar analog of the target phenomenon. To explore this option further, an educational simulation with MERs was developed for chemistry as a demonstration model. One of the MERs designed for this simulation was a "dynamic analogy".

Simulation Design with a Dynamic Analogy

The computer simulation designed for this research was based upon a notoriously challenging concept for chemistry students, Le Châtelier's Principle (*40*, *41*). The latest version of this simulation, described below, can be accessed by contacting the author. The digital interface of this simulation included the following MERs: a symbolic representation of chemical equations, a graphical representation of concentration over time, a molecular animation, and a dynamic analogy of a balance. The interface thus showed several views: a formula view, a slider view, a textual description, a graph view with a prediction mechanism, a molecular view and an analogy view. The formula view represents a chemical reaction. Four different reactions were programmed into the simulation and users could choose which reaction to load. The slider view provides user control to adjust conditions for the closed system, such as the molarity, temperature, and volume. The graph view plots concentrations of the chemicals as the reaction progresses over time. The description view provides text-based information about the products and reactants involved in the reaction. The description view can be switched to a prediction view that then operates within the simulation. First, conditions in the chemical system are adjusted, the simulation is automatically paused, and then users are prompted to answer a multiple-choice question predicting the effects of the changes before the simulation resumes. The molecular view shows a magnified representation of the molecules interacting in the closed system. Finally, the molecular view can be switched to an analogy view. For Le Chatelier's Principle, the analogy view depicts a scale or balance with reactants and products. It is an analogy for a chemical reaction reaching a state of equilibrium.

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The scale or weighing balance analogy was selected for trial in the simulation as it was being commonly employed by chemistry teachers in the region. It had also been documented in the literature by chemistry educators, such as Volland (*28*), who showed how chemical equilibrium can be viewed akin to a weighing balance; the reactants are on the right hand side and the products are on the left hand side. When the system is "balanced", the forward and reverse rates of the chemical reaction are equal. In the simulation, the software designers attempted to simulate this analogy by presenting a dynamic, interactive balance (known as the "dynamic analogy"). Figure 2 depicts the user interface of the simulation used for the research, with the dynamic analogy on the upper right hand side.

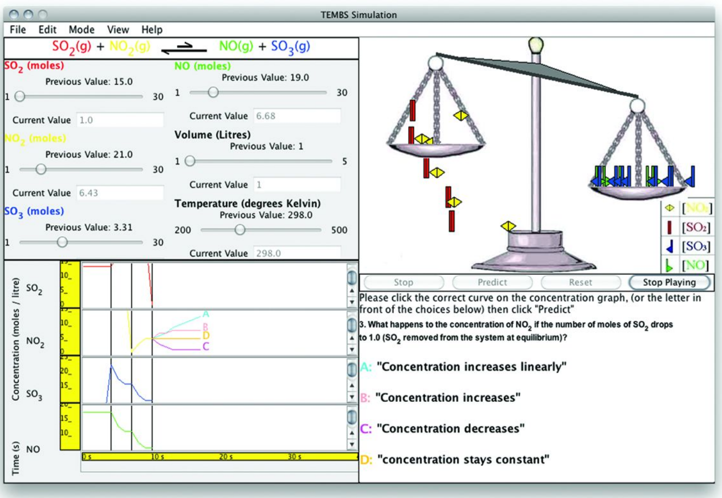

Figure 2. Version one of the user interface with the dynamic analogy. (see color insert)

In Figure 2's dynamic analogy, the colored shapes on the balance or scale represent each of the chemicals in the reaction. Reactants sit on the left side of the balance and products on the right side. For example, to represent the reaction, PCl5(g) ↔ PCl3(g) + Cl2(g), blue triangles are Cl2 molecules, green squares PCl3 molecules, and red composites (a triangle on top of a square) PCl5 molecules. On the screen, all chemicals are shown in the legend on the far left and right. The components of the scale and the shapes are synchronized with a programmable chemical reaction engine built into the simulation. Chemical concentrations are represented by the number of corresponding shapes displayed on the screen and the statement, "Each symbol represents 1 mol of concentration" is placed at the bottom of the analogy view as a reminder. As the reaction progresses, chemicals from one side of the scale can be seen traveling to the other side and transforming into other molecules. For example, when the dynamic analogy in the simulation runs, PCl5, which is represented as a red composite, rotates clockwise and changes into one green square (or Cl2) and one blue triangle (or PCl3). When the rates of the forward and reverse reactions are equal, the sides of the scale are at an equal level, signifying a state of equilibrium. The animation does not stop when equilibrium has been achieved (and the beam is balanced), unless the user presses stop. If a stress is applied to the system, such as an addition of reactants, the system falls out of equilibrium and the beam is shown as temporarily falling out of balance. The system tries to counteract the stress by increasing, for example, the forward reaction rate to form more products. As the product concentration increases, the reverse rate also increases. Equilibrium is re-established when a new balance between reactant and product formation is achieved, and this is shown by the beam achieving balance. In the simulation, the dynamic analogy view, graphical view and the molecular view (not shown in the Figure 2 but can be switched with the analogy view) are coordinated with changes made by the user with the sliders. The analogy is considered to be dynamic as it illustrates that the molecules continuously interact, and the scale shows how stresseses effect the system.

Study 1. Classroom Study on the Use of the Simulation with the Dynamic Analogy

Introduction

The first study explored high school chemistry student interactions with the designed simulation. As a first step, we sought to examine quantitatively if interaction with the simulation and its dynamic analogy feature in particular might contribute to student understanding of Le Chatelier's principle in ways that go beyond more traditional uses of analogy in the chemistry classroom.

Design and Methods

In the first study on this simulation, fifteen chemistry students in grade twelve in a North American public high school were randomly assigned to two groups of academically equivalent students. Both groups had completed their unit on Le Chatelier's Principle, taught by the same chemistry teacher. Both groups interacted with the computer simulation for 90 minutes at individual computer work stations. The first student group interacted with the simulation and associated instructional materials. The second student group interacted with the same simulation and associated instructional materials, except only the dynamic analogy feature was not enabled. Instead, the second group was asked to recall the same analogy to a weighing balance or scale that had been given by the teacher verbally and with static images to both groups at the outset of the study. Both groups responded to the same questions on Le Chatelier's principle, with the first group drawing upon their understanding of chemistry from interaction with

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the dynamic analogy, and the second group drawing upon their understanding of chemistry from the verbal and a pictorial rendering of the scale provided by the teacher. The first group was asked to run the dynamic analogy in the simulation and then respond to the same questions. The second group, instead was asked to recall the scale analogy and to imagine it without running the dynamic analogy view in the simulation. The second group then answered the same questions as the first group about forward and reverse reaction rates and the same prediction question on what happens when additional chemicals are added to the system. The associated instructional materials were pen and paper worksheets of questions that continued to guide students to generate, evaluate and modify their models of chemical equilibrium while following instructional tasks, like the ones above, with the simulation.

An assessment for conceptual understanding of Le Châtelier's Principle was developed and administered to the chemistry students. The assessment contained standardized questions plus questions peer-reviewed by independent content and educational experts in chemistry and chemistry education, respectively. Both groups of students wrote this short answer and multiple-choice question assessment on Le Châtelier's Principle after interacting with the simulation and the associated instructional materials. A pre-assessment was not administered because students were assigned to academically equivalent groups at the outset of the study. (The two groups had an equivalent proportion of high and low achievers based on their performance, the same overall grade averages in chemistry in the past, and had taken the same chemistry courses). The assessment questions generally involved interacting with the simulation and making predictions, drawing molecular models, interpreting graphs of chemical concentrations and their change over time, and constructing explanations at a molecular level. Not all of the instructional materials and assessment questions required student use of the analogy explicitly. The instructional materials and assessments are both available by contacting the author. The assessments were then blind coded and scored by two graders who had an interrater reliability of 99% on them, with the results presented in the following sub-section.

Results and Discussion

The results on the post-assessment revealed that there was a significant relationship between the instructional computer simulation used and the total assessment score, $t(13) = 2.61$, $p < 0.02$. The mean total for the group that used the dynamic analogy in the computer simulation was significantly higher (90%) than the mean total on the test of 68% for the group that did not use the dynamic analogy but instead recalled one. Analysis of the assessment data suggests that student interaction with the dynamic analogy contributed positively to their understanding of Le Chatelier's Principle in a way that went beyond static images and description (*15*, *37*). The findings of Study 1 lead us to believe that dynamic analogies should be further investigated as a design option for simulation technology. Study 2 provides such an investigation.

Study 2. Students' Conceptions in Chemistry with the Dynamic Analogy

Introduction

A second study employed the same demonstration simulation, but this time, explored the ways the use of the simulation might challenge or not challenge students' misconceptions of Le Chatelier's Principle (*29*). All external representations, including analogies, can contribute or impede understanding. Analogies, for example, can inadvertently produce new misconceptions rather than challenge them (*19*, *21–24*). Orgill and Bodner (*30*) shared the potentially positive and negative aspects of analogy use for chemistry teaching. Their meta-analysis of research on analogies in chemistry education identified potentially beneficial effects of analogies on learning. According to their list, analogies contribute to learning by: assisting students in organizing or viewing information from new perspectives, highlighting significant similarities and differences between the analog and target domains, visualizing abstract concepts by providing a concrete example to relate to an unobservable phenomenon, providing a motivational incentive to investigate an unfamiliar scientific concept through a relationship with an interesting and already familiar topic, and fostering conceptual change through a process of replacing older, more erroneous conceptions with newer, more expert-like and accepted conceptions. Orgill and Bodner also recognized potentially negative effects of analogies, such as: redundancy of analogies if the target concept is already well understood, student use of the analogy as a mechanical reflex without questioning or understanding how the analogy represents the target domain, misunderstanding of the representation of the analogy contributing to misconceptions about the target domain, and acceptance of the analogy as the only possible or necessary explanation thereby developing a limited understanding of the target domain. Analogies have the potential to both mitigate and produce alternative conceptions about the target domain, and this research study investigated how this might happen with a dynamic analogy.

Design and Methods

The second study was conducted in a different North American public high school. Two grade 12 chemistry classes with a total of 54 registered students (26 female, 28 male) participated as one group in the study. Both classes were taught the same chemistry content by the same chemistry teacher. The study took place during a one-week time frame towards the end of a unit on chemical equilibrium, using two lesson periods (72 minutes each) for each of the two classes. Students interacted with the entire simulation for a total of 144 minutes and were assessed on their conceptual understanding of chemical equilibrium before, during, and after interactions with it. Before interaction with the simulation, students received traditional instruction on chemical equilibrium, consisting of lectures,

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discussions, labs, and demonstrations. An open-ended pre-assessment was then administered. Students interacted with the simulation individually as part of the regular scheduled classroom activities and completed an activity worksheet while doing so. After this interaction, an open-ended post-assessment was administered.

Assessment tools developed for this study examined student conceptions of chemical equilibrium. In particular, the concepts assessed were when equilibrium is established, when reactions are complete, the appearance of one-sided reactions, equality in amounts, rates and concentrations, and whether chemical processes stop at equilibrium – concepts which have similarities with, and a conceivable potential to be, affected by a scale analogy, graphs, and molecular representations. Three assessments were employed in this study: a pre-assessment, an activity worksheet, and a post-assessment. The pre-assessment was made up of 10 open-ended items, asking students to describe properties of a chemical system at equilibrium, explain why a chemical process happens, and draw molecular representations of a chemical system that has reached or is in the process of establishing equilibrium using pencil and paper. Second, an activity worksheet provided instructions on using the simulation and posed 22 questions as they worked with it. Similar activity worksheets had been developed and used in other classrooms with other high school chemistry students in previous research studies (*31*). In addition to using similar worksheets in classrooms, the activity worksheet questions and tasks were further refined with feedback from a university science student, a chemistry high school teacher with 25 years of teaching experience not affiliated with the project, and another subject matter expert from a university chemistry department. The worksheet questions focused on chemical equilibrium, and students were required to interact with all the views in the simulation in order to answer all questions. Third, a post-assessment was designed to assess what student conceptions may have been altered or what alternative conceptions may have formed as a result of interacting with the simulation. The 10 post-assessment questions were similar in style to the pre-assessment. The pencil and paper post-assessment also contained survey questions about their perceptions of individual external representations employed in the simulation.

Students worked with the computer simulation at individual workstations. Out of the 54 students who participated in the study over the two lesson periods, 46 students completed all three assessments. Statistical means and two-tailed t-test analyses on pre- and post-assessment data were conducted. All quantitative and qualitative data, such as student drawings, were analyzed for their accuracy according to the scoring guide. To determine inter-rater reliability, the worksheet responses and assessments were evaluated by two graders: a chemistry subject matter expert and a research assistant. The graders met to evaluate sample responses together, discuss heuristics for marking, and clarify the marking scheme, resulting in an overall inter-rater reliability of 89%. To take into account any discrepancies, questions that were not graded the same were discussed in order to achieve consensus. If differences remained after such a discussion, scores were averaged. Statistical inferences were drawn from an analysis of data using a statistical software package. While causal outcomes were not sought for isolated MERs, hypotheses were generated about the ways the external representations, including the dynamic analogy, might have contributed to the findings.

Results and Discussion

Four findings are reported from this analysis here. The first finding revealed that significantly more students understood the forward rate of a chemical reaction on the post-assessment compared to the pre-assessment. Students were asked to consider a system at equilibrium: suppose more of the reactant chemicals are added to the system. a) What will happen to the rate of the forward reaction? Why? b) What will happen to the rate of the reverse reaction? Why? A two-tailed t-test analysis of the marks indicated that the difference between the means was significant at the $p < 0.05$ level ($p = 0.0138$). Students correctly identified that the forward rate instantaneously increases due to the increase in the concentration of reactants after interaction with the simulation. On the pre-assessment, 30 out of 46 students earned more than one point (i.e. one point was awarded for identifying correctly that the forward rate increases and an additional point was awarded for a correct explanation) while 43 out of 46 earned more than one point for the same question on the post-assessment. Responses for the reverse rate question, however, remained relatively unchanged before and after interaction with the simulation and its instructional materials (15 of 46 students earned more than one point on the pre-assessment while 16 of 46 students did so on the post-assessment). The most common conception held by students on the reverse rate question was that an increase in the forward rate would result in an immediate, opposite effect in the reverse rate. Given comparisons of the pre- and post-assessments, interactions with the simulation alone did not generate this misconception, but it is possible that an already existing conception remained unchallenged by the MERs available, including the dynamic analogy.

A second finding is that students expressed models before equilibrium improved. Here, students were asked to draw how molecules would appear in a closed system before equilibrium was reached. A two-tailed t-test analysis indicated a statistically significant difference between the means ($p=0.03$, $n=46$) of this pre- and post- assessment question. Eighty-three percent (38 of 46) of students on the pre-assessment and 91% (42 of 46) on the post- assessment question were able to draw molecular models with an appropriate distribution of molecules and the ratios of molecules needed to corroborate their explanation of the before equilibrium state. The overall significant improvement in their before equilibrium models from pre- to post-assessment could be attributed to interaction with the simulation and to hypothesize more specifically, the molecular view in the simulation. This particular view in the simulation shows how molecules interact in a closed system throughout the process of achieving equilibrium. Students' drawings were consistent with those shown in the molecular view. It is plausible that the molecular view offered to students a demonstration of how to represent a closed system.

A third finding was that students were not able to accurately draw a model of what happens at equilibrium and this finding appeared exacerbated after interaction with the simulation ($t(45)= 2.77$, $p = 0.008$). In addition, fifty percent (23 of 46) of students on the pre-assessment and 46% (21 of 46) on the post-assessment depicted equal numbers of each molecule at equilibrium in their drawings (see Figure 3), that did not correspond with their before equilibrium drawings. This

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sudden equality of numbers of moles in the chemical reaction at equilibrium may have occurred with students who were confused about what equilibrium equalizes - not numbers of moles or concentrations but rates of reaction.

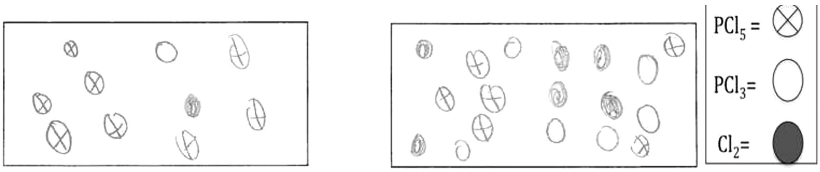

Figure 3. Student drawing of equilibrium before (left) and after (right). Reproduced with permission from reference (29). Copyright 2011 Research Center for Educational Technology.

Interaction with the simulation did not appear to challenge students' misconceptions regarding what happens "at equilibrium" according to pre-post assessment comparisons. Animations do not stop automatically at the point of achieving equilibrium, and the computer simulation as a whole does not further clarify when equilibrium has been reached with audio or narrative cues. Of all the views contained within the simulation, arguably the graph view most clearly depicts when there are no further net changes in concentration with the passage of time. The analogy and molecular views (which are both dynamically linked to the graph view) depict multiple symbols representing molecules in motion and may be challenging to interpret as representational devices without additional guidance or cues.

A fourth finding in students' drawings was referred to as compartmentalization. Forty-three percent (20 of 46) of the students compartmentalized or grouped molecules in a non-uniform distribution pattern on the pre-assessment drawings while 30% (14 of 46) did so in the post-assessment drawings. In these drawings, molecules were grouped into rows or columns. Another variation in this diagrammatic trend showed all reactants on one side and all products on the other. Molecules may have been shown in a compartmentalized fashion because the cognitive load in doing so was lower and made the molecules easier for students to count. It is also plausible that drawing the molecules in a mixed, heterogeneous manner may not have been important to the students or perhaps it did not occur to them. The simulation includes a molecular view that portrays a reaction in a closed system. Molecules of different types are scattered amongst each other in a heterogeneous manner and remain randomly distributed for all chemical reactions and during all phases of chemical reactions. It is plausible that through observing the molecular view, students learned that it was more appropriate to show molecules "mixed up" in the drawings on the post-assessment.

In summary, several of the findings reported showed statistically significant improvements in students' explanations and drawings of chemical equilibrium. The findings of this second study suggested that overall, graphs, analogies, symbols and animations of molecules in motion are a set of digital representations

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that has potential to support understanding in chemistry. While the second study did not seek to examine the effects of the dynamic analogy in isolation from other representations, the dynamic analogy was hypothesized to have contributed to the pre-post gains.

A final post-assessment question in the second study was a 5-point Likert response question asking students to rate how helpful they found the simulation as a whole and the various parts of the simulation. A rating of 5 corresponded to "very helpful" and 1 to "very unhelpful". Mean ratings ranging from 3.93 to 4.68 suggested that students generally perceived all parts of the simulation were helpful to their understanding of chemical equilibrium. The simulation's graph view appeared to be most favored by the students, receiving the highest mean score and the largest cluster of ratings near the 5-rating. The simulation's analogy view was also strongly received with a mean rating of 3.95. It was considered slightly less helpful than the graph view but more helpful than the molecular and other views according to the student respondents. Graphs depicting the change in concentrations of reactants and products during equilibrium may have been considered more helpful than the analogy view because the graphs more clearly compared concentrations in the reaction with the use of color coded lines and afforded the capacity to view minute changes in concentration over time. This result may provide impetus for designers to also graph changes in the rates of reactions and changes in the amounts of reactants and products in the simulation. Molecular representations or nano-scale views that convey the more unobservable aspects of science tend to be more common in chemistry simulations than analogy views (*32–34*), and continued assessment of this representation, along with the others, would be warranted in future studies on simulations. Examining how visual and verbal cues may support student interpretation of the MERs might further enhance student understanding with simulations

To conclude this section on non-standard external representations, research on dynamic analogies is ongoing. The initial findings of these studies leads one to recommend continued exploration of dynamic analogies as a design option for computer simulations in chemistry education. Perhaps more significantly, the development and testing of dynamic analogies as a non-standard representational device underscores the potential for a program of research in educational technologies that borrows powerful extant teaching strategies from science education.

Part Three: T-GEM as a Pedagogic Design for Classroom Environments

Introduction

Design can not only be considered as encompassing the design of the simulation and its interface (as in the first section of this chapter) but also the design of the pedagogic methods that integrate this technology in the classroom (as in this section). The second section of this chapter synthesizes existing research on the T-GEM method as a possible design for integrating computer simulation technology. Since none of our existing simulation technologies in chemistry tutor the student independently, it is vital for educators and designers to consider how simulations can be effectively integrated in teaching and the pedagogic design of activities using this technology as suggested by this part of the chapter.

T-GEM stands for Technology-enhanced Generate-Evaluate-Modify. This pedagogical design is a departure from more traditional approaches to teaching chemistry in classrooms (with or without digital technology) that tend to involve providing a lecture consisting of instructor definitions and some explanation of the phenomena, instructor demonstration of the phenomena, and instructor modeling of problem-solving. T-GEM emerges from an in-depth, 3-year analysis of an undergraduate chemistry teacher's pedagogical design that integrated a suite of computer simulations known as Chemland (*9*, *38*). Chemland, developed by Bill Vining and his working group, houses a number of simulations in its suite that represent lab information, according to the suggested schematic in Figure 1. For example, a screenshot of Chemland's calorimetry simulation from Version 5 is shown in Figure 4.

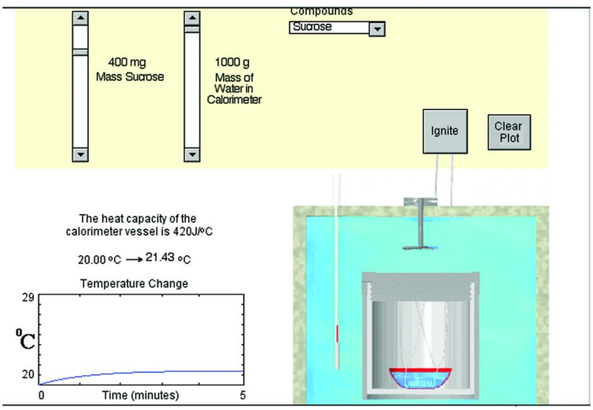

Figure 4. User interface of Chemland's calorimetry simulation, Version 5 (38). Courtesy of Bill Vining. (see color insert)

Design and Methods

The context for research on the pedagogic design of this classroom that employed simulation technology was an introductory undergraduate chemistry classroom in a large North American public university. This class had a department-wide, introductory chemistry syllabus, text, an electronic homework system, and a resource center with computers. The classroom contained computer stations for undergraduate students. The undergraduate students were organized in pairs or groups of three at these terminals. Each terminal was equipped with the Chemland suite of simulations. The syllabus topics for the general introductory chemistry course were atomic structure, molecular structure, organic chemistry,

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gases, liquids, solids, properties of the elements, chemical reactions, energy, and reactivity. A one-semester (13-week) introductory chemistry course was offered to science and nonscience majors every year for the three year duration of the research on it. The chemistry teacher for this course, who was a faculty member at a university, had received a teaching award, was identified as a leader in chemistry education within his department and had published both chemistry bench research and textbooks for undergraduate chemistry students. In an interview about his pedagogical goals for students in the course and his approach to instruction, the teacher stated: "I want them to learn chemistry, [but] I don't want them to just understand the concepts—I want them to understand where to get the concepts and where they come from." To accomplish this, the teacher designed an approach to instruction that involved promoting understanding chemistry at the molecular level through inquiry. This study extracted this approach and its possible contributions to students' capacity to do chemistry (*31*). As well, a second part of this same study examined specific heuristics for teaching chemistry with simulations (*35*). The data and results for both are presented collectively as pedagogic design.

Multiple sources of qualitative and quantitative data were collected in this research study. Sources of data over a 3 year period of data collection included: classroom observation notes, a chemistry education survey, transcripts from in-depth problem-solving sessions with pairs of students and their teacher, and a teacher interview. Data was collected every year, for 3 years. The data collected annually were: 20 sets of classroom observation notes (including classroom handouts), 10 classroom observation rubrics, and responses from a chemistry student survey (n=24). In addition, in the final year of data collection, six 2-hour, in-depth, problem-solving sessions with students from the class (n=12) and one hour of transcribed teacher interviews before and immediately after one of the semesters of observation were obtained.

Classroom observations were conducted by three trained observers. Teacher–student interactions were recorded by observers as notes using a detached open-ended narrative method. Memos summarizing interactions were then written and shared among observers after observation. Observations were further coded in a classroom observation rubric. A classroom observation rubric was designed to record frequencies of teacher and student behaviors according to categories of activities associated with inquiry. The rubric was piloted across introductory science courses at three different institutions prior to this study and underwent significant peer review in multiple debriefing sessions after in-class observations and after viewing videos of classroom interactions. Inter-rater reliability on the use of the classroom observation rubric by the three observers was 84%.

In-depth problem-solving sessions were designed to document student learning by capturing and elaborating on students' model-based inquiries in rich detail. In these in-depth sessions, the teacher taught a lesson to a pair of students in a study space adjacent to the classroom. Because a person can express ideas about a phenomenon in a variety of ways, the students were prompted by the researcher to say out loud what they were thinking, and they were provided with sheets of paper in the event that they wished to draw. The sessions were recorded by video and audio and were transcribed afterward. The session activities were typical classroom activities. More than a third of the students (n=12) enrolled in the course participated in the 2-hour in-depth problem-solving sessions.

A chemistry survey with a 5-point Likert scale was also administered at the end of the semester. The survey was designed to gauge introductory chemistry students' perceptions of their learning experiences in science and chemistry. A process of refining the survey over a year prior to the final semester was followed to strengthen reliability, and this process included pilot testing, peer review, and student focus group and member checking. These classroom observation rubrics and surveys can be obtained by contacting the author.

Results and Discussion

A Pedagogic Design of Instruction: T-GEM

Classroom observations from this research elucidated a detailed, complex set of interactions among the teacher and students as they were engaged in conceptual activities with the computer simulation (*31*). The results of this analysis revealed a pedagogic design that followed a general three phase pattern of instruction. Phase 1: the teacher helps students generate (G) ideas; Phase 2: the teacher works with students to evaluate (E) their ideas, and Phase 3: students modify (M) their ideas individually and as a class. Phases 2 and 3 cycled until students expressed a scientifically accurate model of the concept. On average, in one period of class, the teacher engaged in this pedagogical approach two times, for a total of 52 times across 11 different topics in chemistry. The teacher was observed consistently using computer simulation technology (T) in every phase of what was termed the GEM cycle (eg. T-GEM). Computer simulations were thus used at least twice per class.

For an example of a typical classroom teaching episode observed with the computer simulation, a lesson on intermolecular forces is relayed here in the results section. In the lesson, the teacher (T) began this new topic first with background information defining vapor pressure and boiling point:

> T [B]oiling point is defined as the temperature at which this curve [referring to a graph of two substances' vapor pressure and temperature] reaches 760 [mm Hg]. 760 is atmospheric pressure, so when the vapor pressure reaches atmospheric pressure, that's when things boil.

When asked in the interview about how much background information is enough, the teacher indicated that students need, "[B]ackground enough to know what the data is and what it means." The data being referred to were data on vapor pressures and boiling points of organic compounds. The teacher went on to say that, "[T]he thing that they should not know before they start looking at it [the simulation] is what the overall relationship and guiding principles [under investigation] are." In fact, the teacher discouraged students from reading the text beforehand. Providing background information lasted, on average, less than 5 minutes at the beginning of class.

Phase 1. Students Generating (G) Hypotheses in Chemistry with Computer Simulations

In the first phase of instruction (G), the teacher was observed asking students to generate hypotheses regarding relationships between variables. After providing background content information, the teacher had students work in pairs or groups of three to gather information from two Chemland computer simulations. The teacher stated that, "The time to be able to do it [introduce a computer simulation] is [when students] know what it is they're looking at. They need to know what the information is telling them in each data point by data point instance." The teacher typically identified key variables for students to examine from the simulation and asked students to compile information about the relationship between the identified variables. In the lesson on intermolecular forces, the teacher (T) asked students (S1, S2, S3,…) to gather information from a Chemland computer simulation (Version 5) on the vapor pressure of different compounds. This particular simulation would be classified as lab information according to Figure 1, as it depicts an animation of two flasks each containing a compound and a pressure gauge, a slider to manipulate temperature, and a graph of pressures vs. temperature. The italicized portion below in the transcript of teacher-student discussion with the simulation indicates the teacher action to generate a rule concerning the relationship between two variables, molecular weight and boiling point.

> T So let's go ahead and just look at what the boiling points are for these things [ethanol and methanol]. So ethanol's between 78 and 79 degrees—its boiling point [pointing to the vapor pressure simulation]. So methanol is between 64 and 65 degrees [using a graph in the vapor pressure simulation to locate approximate boiling points].
> S2 Uh, huh.
> T Does that make sense? So *what do you think the relationship between molecular weight and boiling point is?*

Responding to this teacher action, the transcript below shows students (S1 and S2) using the simulation to generate (G) an initial relationship:

> S1 [Pointing to the simulation's graph of vapor pressures] As the molecular weight increases, the boiling point also increases because for ethanol it's more, it has a greater molecular weight and the temperature it takes for it to boil is between, did he say 70 and 80?
> S2 Uh, huh. Something like that. Well we can check.
> S2 Yeah, between 78 and 80 [referring to simulation's graph].

Following the generation of a rule concerning a relationship in chemistry, students were regularly asked to explain their reasoning to the teacher. For example, the transcript below shows the teacher asking students to explain the relationship between temperature and vapor pressure and students' explanations of why methanol and ethanol have different vapor pressures.

T Okay so I have another question then. So as the temperature goes up, vapor pressure goes up you said. Come up with an explanation for that. Why as the temperature goes up does the vapor pressure go up?
S4 Methanol would be lighter and as we figured out from the first part, if it's lighter mass, the velocity goes up and the amount of gas goes up before the vapor pressure goes up, so methanol, since it is lighter, would go up, should go up quicker, which apparently it does on the graph.
T So okay.
S3 Because like I never thought about, like I didn't connect the mass to the vapor pressure kind of….I'm assuming because it's [ethanol], a longer chain, the bonds would be weaker. I'm not sure, because one of the OH pulls the end of each one; pulls like electrons or pull something over to like their side the OH side. And so therefore bonds towards, like the end, like the CH3's, [would] be weaker.

In this transcript, students explained how methanol could have a higher vapor pressure than ethanol using mass as the critical predictor of vapor pressure. S4's explanation involved reasoning about the behavior of molecules, hypothesizing that molecular "velocity goes up" as temperature increases, and lighter molecules "should go up quicker." S4 coordinated this theoretical idea that lighter molecules "should go up quicker" with data from a graph on temperature and vapor pressure that was available as part of the data set, claiming that "apparently it [methanol] does on the graph." The mass property of molecular compounds was the most prevalent feature of students molecular models used to explain the relationship between temperature and vapor pressure of molecules. S3, however, remained unconvinced by a "mass model." S3 proposed an alternative molecular model to explain the different rates of vaporization between methanol and ethanol. It can be described as a model of molecular structures containing an intramolecular pull or an intramolecular force. The molecular structure of ethanol was postulated by S3 as having weaker bonds because it is a longer chain. To explain why longer chains would have weaker bonds than shorter chains, S3 revealed a model where one of the hydroxyl ends of the molecule pulls electrons within the chain toward itself, weakening the remaining bonds. This intramolecular pull to one end within a molecule is the reason why, according to S3, ethanol has a lower vapor pressure than methanol. Students expressed various models of molecular structures as they were engaged in generating hypotheses in this first phase of T-GEM.

In an effort to explain the initial relationships they had generated, the analyses of videos revealed that with the simulation running, students were diagramming, pointing to, and gesturing over the diagrams they had drawn on paper, and also were offering spontaneous analogies themselves. Examples of the analogies students expressed to explain the behavior of molecules included the following: sumo wrestlers and marathon runners running a race (to represent molecules of large and small molecular weights), skating (to represent how molecular bonds break), and dropping a ball on a soft and hard mattress (to explain molecular movement during vaporization). Asking students to explain relationships appeared to spur students' reasoning about what was happening at the molecular level and their spontaneous use of analogies. Although students

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expressed models of molecular structures were not entirely scientifically accurate, it was also observed that the teacher refrained from pointing out problems with the relationship they had generated in phase 1 or their explanatory models at this stage.

Phases 2 and 3. Students Evaluating (E) and Modifying Hypotheses (M) with Computer Simulations

After generating (G) initial hypotheses regarding the relationships among molecular mass, molecular speed, vapor pressure, and boiling point in phase 1, the teacher asked students to evaluate (E) these initial hypotheses in light of new information, as revealed by interaction with a third simulation on organic compounds and boiling points. For example, the teacher stated following phase 1 of instruction, "We want to use this [a third simulation] to see if your trend there [referring to a hypothetical relationship students had constructed: 'As molecular weight increases the boiling point increases'] actually works for more than say two compounds." In this boiling points simulation (a lab information simulation, according to Figure 1), students are able to select the alkyl and functional group of a compound and view a space filling model of it along with its boiling point. Students can also generate a graph of boiling points by molecular weight. Using this simulation, students were able to plot a graph of selected alkanes and functional groups unique molecular weights and boiling points. Students expected that in general, boiling points would increase as molecular weights increased. This trend was evident in most cases, but compounds with functional groups that had the capacity to hydrogen-bond, such as hydroxyl and amine groups, had anomalously high boiling points for their molecular weights. The following excerpt shows two students' responses to this anomaly on the simulation:

S4 Why does this thing appear [points to the methyl hydroxide data point in a boiling points versus molecular weight graph on the simulation]?
S3 Do you mean that? Hydroxyl? [points to the simulation's graph]
S4 Hydroxyl…
S4 It doesn't follow the trend.
S3 It boils high for its weight because chlorine boils lower and that's much, that's heavier.
S4 The hydroxyl still boils at a higher rate. It doesn't follow the same trend as the other.
S3 These others increase almost linearly [referring to the graph]. Almost in a line, but hydroxyl's kind of out, at its own boiling point.
S4 Hydroxyl's right here and it's.
S3 Right it's far away.
S4 Abnormally high.

The teacher asked for an explanation for the "abnormally high" boiling points. At this point, students became engaged in evaluating the empirical consistency of their initial ideas and coordinating their theoretical models of molecular structures with this new information in an attempt to explain the anomalously high boiling points of several compounds. Students subsequently expressed models of molecular structures that emphasized differences in molecular mass, electronegativity, shapes of the molecular compounds, and "bonds" between two hydroxyl groups (as described in the excerpt below):

> S4 Okay. Wouldn't the, on this one say, remember how we were talking about how there would have to be a bond between things in a liquid to hold them together as a liquid?
> S3 Uh, huh.
> S4 What do you think about the bond; what kind of bond there would be between two hydroxyls?
> S3 Two hydroxyls?
> S4 Would it be a stronger bond than say between two chlorides or two bromides?
> S3 Most likely because, between two hydroxyl groups? Between an OH and an OH?
> S4 Like between an OH and an OH. (S4 draws a double bond between two hydroxyls on a piece of paper).

The idea of a "bond" between hydroxyls, although not scientifically accurate, suggested that students were postulating a hidden causal factor, in this case, a bond, to explain the anomalously high boiling point. Students had not included this factor in their explanations nor drawn it prior to this lesson. The above transcript was the beginning of a student discussion on intermolecular forces to explain differences in boiling points. Using a computer simulation and a set of guided activities involving discrepant information, the teacher was able to provoke an evaluation and modification of students' initial molecular models and the set of original relationships they had proposed.

All students in this lesson were able to eventually postulate the idea of a "bond" as the best explanation for the puzzling data by the conclusion of the instruction. In the last phase of T-GEM, students were subsequently observed modifying (M) their molecular models to include an intermolecular hydrogen bond. With their modified models of molecular structures, students were able to predict a new case, the effect of molecular weight on the boiling points of two new compounds, water and benzene. Students were able to make predictions regarding different compounds' boiling points using their newly revised molecular models, suggesting that students' models were now enriched with new explanatory power. Finally, students enrolled in this course in previous years produced the greatest pre–post gains on a general test on skills at scientific inquiry ($p<0.05$; $n=198$) and highest overall post-test scores compared with other introductory chemistry and general science classes (*36*). Furthermore, in this iteration of the course, ninety-six percent of this class successfully passed their department-wide exam.

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Role of the Simulation and the Pedagogical Design of Classroom Activities

The role of the simulation was to support specific phases of instruction in T-GEM. Classroom observations and in-depth problem-solving sessions illustrated that the simulation appeared to support chemistry instruction by affording students and teachers with the capacity to compile information between variables. This information was used by students to generate initial relationships relatively quickly, push values to extremes or, in increments, and to assess the scope of the relationship they had developed. In addition, Chemland provided an environment to make comparisons between data and draw attention to visual patterns and contrasts using graphs and animations. Students were also observed testing their assumptions, dynamically regenerating graphs, and viewing graphics at the molecular level with this suite of computer simulations. Simulation technology also appeared to afford students with the capacity to engage in multiple GEM cycles in one classroom period, likely beyond what could have been accomplished in the laboratory.

A student survey asked students their perceptions of the impact of the computer simulation on their understanding of chemistry and problem solving (*35*). The majority of students agreed that, “The use of simulations in class has contributed to the development of my ability to critically analyze a problem in chemistry” (75% agreed, 4% disagree; 21% neutral; n=24). They also reported that, “An important advantage of the computer simulations is that they make unobservable processes in chemistry more explicit to me” (90% agreed, 5% disagree; 5% neutral; n=21). Further, students revealed that, “The computer graphics of molecular structures used in lecture contributed to my learning in this course in a way that went beyond what I learned from the pictures used in the text” (76% agreed, 19% disagree; 5% neutral; n=21). Finally, the computer simulations did not detract from learning: “When using computer simulations in class, if I do not understand the concept before hand, the in-class simulation compounds my confusion instead of clarifying the concept” (14% agreed, 72% disagree; 14% neutral; n=21). The computer simulation appears to have contributed positively to student learning according to them.

While the vast majority of students surveyed reported that they could complete the activities involving the computer simulation, 76% of surveyed students agreed with the statement that: “Teacher guidance is necessary for the effective use of the simulations” (14% disagreed, 10% neutral, n=21). Out of seven possible choices in a survey ranking question, the top three student-ranked choices for where the greatest learning happens for them was (in order): teacher discussion with the students during class, simulations, and their electronic homework system (n=21). In a second ranking question on the survey, a majority of surveyed students (n =24) ranked the independent use of simulations outside of class in one of their bottom three choices out of nine choices to “rank where the greatest learning happens for you in chemistry.” Finally, these collective findings suggest that the pedagogical design of classroom activities played an important role in learning with simulations. This research further contributes to a larger discussion of what becomes designed when we design simulations and suggests that the design of instructional activities, such as T-GEM, be considered alongside the research and design of the simulations themselves.

Conclusions and Future Directions for Research on Educational Design

In conclusion, in this chapter, computer simulations are positioned as a unique digital technology from other interactive tools that, in chemistry education, may be typified in one of several sub-categories based on their functionality. Figure 1 suggests several such sub-categories of simulations. The significance of delineating types of simulations is to begin to capture the different types of simulations that have emerged in our field for purposeful and often distinguishable pedagogical aims. Despite the array of simulations available in chemistry education and their distinguishable characteristics, they also tend to share several features in common, including the use of multiple external representations or MERs. A comparison of MERs, as suggested in this chapter, is helpful to putting forward new design directions for research on them. Two possible directions for the future of educational design in computer simulation technology were put forward in this chapter, including the design of the simulation's interface and secondly, the design of pedagogic methods that integrate this technology. An external representation, the dynamic analogy, was considered in the research presented here as a non-standard design option for MERs. Findings from two specific studies on the dynamic analogy, suggested that it may serve as a viable alternative external representation that can support student understanding in chemistry. While further research on dynamic analogies are necessary, this representation is a meaningful departure from traditional external representations in chemistry (e.g. symbolic, sub-atomic, macromolecular). Perhaps more significantly, the development and testing of dynamic analogies as a non-traditional representational device underscores the potential for a program of research in educational technologies that borrows powerful extant teaching strategies from science education. Finally, through research on a coordinated use of a computer simulation in a chemistry instructional environment, the author suggests how computer simulations can be used productively in the classroom. A multi-step approach to using computer simulations in chemistry was revealed from a third study of a classroom that employed this technology. There are relatively few multi-step approaches that integrate digital technology in science education, and almost none reported for chemistry education. Known as T-GEM, this approach incorporates particular phases of instruction and activities that regularly and fully integrate computer simulations. Taken collectively, both approaches to design, the simulation and the instruction, constitute possibilities for the future of educational research on this technology.

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Chapter 15

Designing Analogy-Based Simulations To Teach Abstractions

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Animations, simulations and visualizations are playing an increasingly important role in chemical education. A powerful use of such tools is to give students experience at the particulate level of chemistry by depicting collections of molecules. In this chapter, however, the use of different, analogy-based simulations is considered as a means to help students learn abstractions that lie at the core of chemical reasoning. Rather than depict atoms and molecules directly, the presented simulations involve boxes, steps, and bouncing balls, which were chosen because of their familiarity to students and their ability to represent chemical systems by analogy.

In this chapter, it is argued that appropriately designed analogy-based simulations have the potential to help students learn the important abstractions that are used by experts to organize their domain-specific knowledge. Before presenting guidelines on how such simulations may be designed, necessary background information is presented. This includes a brief review of analogies and their use in science education, a description of analogy-based simulations and their potential benefits, as well as an overview of abstractions and their importance in expert knowledge structures.

The chapter concludes with guidelines on how to create analogies and analogy-based simulations, particularly those that use multiple external representations in order to address

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abstractions. The presented concepts are illustrated using examples of analogy-based simulations that were created to teach the thermodynamic abstractions of energy landscapes, thermally-activated processes, and entropy-driven reactions.

Introduction

Over the last thirty or so years, analogies have enjoyed increasing attention in both the education and psychology literature. Within the realm of science education, in particular, the study of analogy usage in texts and in classrooms (*1–8*), as well as advocacy for the use of analogies to teach difficult concepts (*9–14*) has been significant and influential. Those who specialize in chemistry education have also taken an interest in the use of analogies to teach chemical concepts (*15–19*). Simultaneously, educational psychologists and cognitive scientists have been building theories of how people use and understand analogies (*20–27*), which has provided additional guidance to those interested in using analogies in educational contexts. In sum, we now know that when used in appropriate ways in the teaching of well-suited topics, analogies can provide a powerful means to enable students to understand difficult subjects. Furthermore, research is continuing to refine our understanding of which subjects are well-suited to treatment by analogy and how to best present analogies in educational settings.

Over approximately the same span of time as analogies have come to prominence, computer-based visualizations and simulations have also undergone a transition from uncommon to ubiquitous. This has occurred in many fields of science and engineering, though it has been perhaps most pronounced in physics and chemistry. In chemistry education, as computers have become cheaper and increasingly powerful, visualizations have progressively replaced physical models. Furthermore, the growing body of research in student misconceptions has identified many areas of difficulty that can be traced to deficient understanding of stuctures and processes at the molecular level (*28*), providing impetus to create simulations of these structures and processes for students.

Finally, research into the nature of expertise has uncovered that experts' knowledge is structured differently from that of novices. In particular, experts' domain-specific knowledge is organized in ways that reflect the deep, abstract connections within the discipline, with seemingly disparate systems or concepts grouped around the archetypal abstractions of which they are instances. As a consequence, it may be advantageous to directly instruct students on the abstractions used by experts, in order to help them along the path toward expertise.

In this chapter, we argue that there may be compelling benefits for the marriage of analogy and simulation, particularly in the service of conveying abstractions, and we hope that, through this contribution, we will both equip and motivate others to think about ways to deepen student understanding through analogy-based simulations.

The "What" and "Why" of Analogy-Based Simulations

What Are Analogies?

Before we discuss analogy-based simulations, it is first necessary to clarify what is meant by the term "analogy". Analogies come in many forms but, fundamentally, they compare one concept or item with another. Vague analogies might take the form "A is like B", where A and B each represent a concept or object. In this case, how exactly A is like B is not specified and remains open to interpretation. A more specific analogy might take the form "A is like B in that…". Such an analogy explains the manner in which A is like B. In the cognitive science literature, stating that two physical objects resemble one another visually is categorized as a statement of "mere appearance", rather than an analogy (*20*). Analogies, on the other hand, claim similarity between objects on a deeper basis, such as similar relationships between constituent components.

Simple analogies of the form "A:B::C:D" clearly display analogies' focus on relationships. These analogies assert that two pairs of objects or concepts, (A,B) and (C,D), share identical relationships. That is, the relationship that A has to B is the same as the relationship C has to D. These analogies make no claim that any kind of similarity exists between A and C or B and D. Rather, they focus on the similarity of the A-B relationship to the C-D relationship.

While such analogies involve one shared relationship, more useful and powerful analogies typically involve many shared relationships. When drawing an analogy between two concepts or systems of objects, it is unlikely that all internal relationships will be shared; however, good analogies will involve the sharing of many, particularly high-level, relationships (*20*). A concept or system can be modeled as a group of interconnected nodes, where the nodes represent sub-concepts or objects belonging to the system and the internodal connections represent relationships. Creating an analogy, then, involves aligning the structure of the nodal network of one concept to the structure of another. Gentner (*20*) coined the terms "structural alignment" and "structure mapping" for this process. In this process, the identity of each node is not important; rather, only the topology of the network and nature of the represented relationships are relevant.

In education, analogies are used to teach students about an unfamiliar concept, system, or process by means of its relationship(s) to a familiar concept, system, or process. In this usage, the unfamiliar concept is typically called the *target*, though some researchers call it the *topic* (*5*, *29*). The familiar concept goes by many different names in the literature, including *base* (*20*), *source* (*30*), *analog* (*11*), and *vehicle* (*5*, *29*). In this chapter, we will use the terms *base* and *target*, respectively.

While various different approaches to teaching with analogies have been put forward in the literature (*10–12*, *31*), they generally share the idea that the "mapping" between the base and the target should be made explicit by the instructor. This means that, for each of the base's elements (objects, relationships, etc.) involved in the analogy, the corresponding element in the target should be clearly identified. Furthermore, elements possessed by the base and the target that are not involved in the analogy should also be clearly identified, so students do not

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try to create a mapping where no appropriate mapping exists. This helps students to understand the extent of the analogy's applicability and where it breaks down.

What Are Analogy-Based Simulations?

Now that we have considered analogies and how they may be used in education, let us turn our attention to analogy-based simulations. Here, we will consider what analogy-based simulations are and provide an illustrative example. This will be followed, in subsequent sections, by discussion of how analogy-based simulations might be useful in chemistry in general and how they could be used to teach abstractions, in particular.

Analogy-based simulations are simulations that do not directly depict atoms or molecules; rather, they simulate a different physical system that relates to a chemical system or concept by analogy. In the simulations we have created, we have chosen to make analogies between chemical systems and familiar objects from students' everyday experiences, including boxes, steps, and balls. Because students are not typically experienced in reasoning qualitatively about chemical systems, our goal was to leverage their experience with the world around them to help them better understand chemical concepts.

For example, the simulation shown in Figure 1 was designed to support a curriculum sequence aimed at helping students understand a few important concepts related to thermodynamic states and their populations: 1) the higher the energy of a given state is in relation to that of another possible state, the lower its population will be 2) for a series of states with linearly increasing energy, the state populations decay exponentially 3) raising the temperature of a system increases the population of high energy states up to the limit that all states are equally populated. These statements, of course, only apply if the degeneracy of all states is equal.

To illustrate these concepts, we put non-interacting balls on a vibrating staircase. Table I details the analogical correspondences between features of the staircase system and chemical systems. While students may have never experienced a *vibrating* staircase, they have all experienced a staircase and balls' or other objects' tendencies to fall down steps. The effects of vibration, while possibly unclear in an unsimulated analogy, are clarified by means of the simulation.

For the learning objectives associated with this simulation, the main quantities of interest are the vibration amplitude (temperature) and the difference in height between steps (energy difference between states). Control over these two quantities is provided to students through the sliders in the simulation user interface. These sliders can be used by students to complete tasks described in the curriculum, that ask them, for example, to change these quantities independently and observe the response of the system. When completed, the curriculum will then ask themto rationalize what they observed and compare and contrast it to a real chemical system. For example, although the step height increment can be adjusted in the simulation, the difference in energy between two states in a real chemical system is not adjustable.

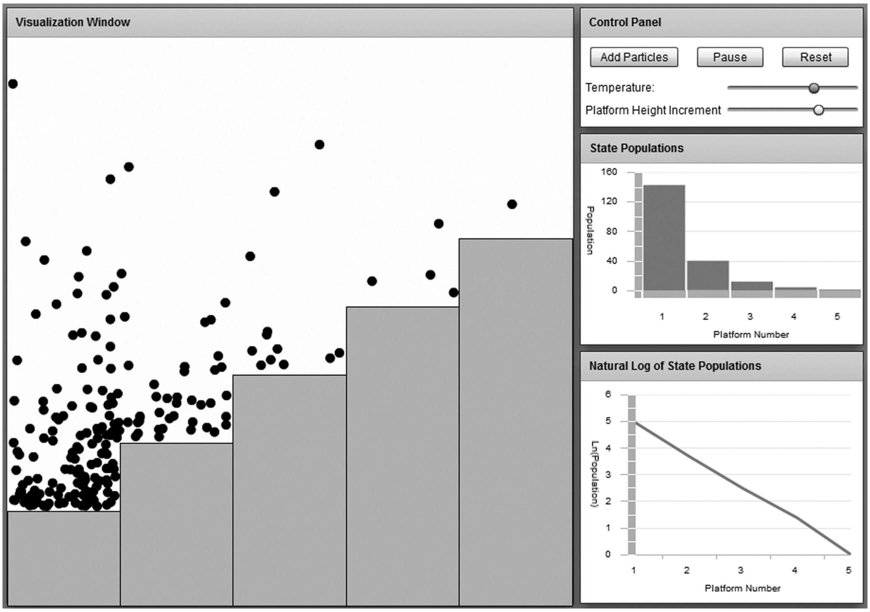

Figure 1. Balls bouncing on a vibrating staircase as an analogy for the population of states in a chemical system.

Table I. Analogical Correspondences Between Staircase and Chemical Systems

Feature of Chemical System	*Representation in Staircase System*
(sub)System	Ball
State	Step
State energy	Step height
Temperature	Vibration amplitude
State population	Number of balls above a step

In addition to the simulation itself, the user interface also provides two further representations of the state populations. Both of these representations are meant to clarify properties of the Boltzmann distribution. The exponential decay associated with the Boltzmann distribution is displayed in the bar graph at top, while the fact that the natural log of an exponential decay takes the form of a downward-sloping line is shown in the line plot at bottom. Thus, in addition to observing that fewer balls occupy higher platforms when the difference in energy between states is increased, students may also observe that such an increase causes the slope of the line at bottom to become steeper, while increasing the temperature causes the slope to become shallower.

While using a simulation to illustrate these concepts is not strictly necessary, we believe that it provides a more compelling and memorable learning experience than simply looking at an equation or a graph. Furthermore, many students are not skilled at interrogating an equation or graph in order to construct a general, qualitative understanding of what the graph or equation represents (*32*). Providing multiple representation of the system – both a simulation and associated graphs – may make it easier for such students to interpret the graphs and construct a qualitative understanding of the important functional relationships that govern system behavior (*33*).

What Are the Potential Benefits of Analogy-Based Simulations?

We are not aware of any studies that have compared the efficacy of analogy-based simulations to analogies presented in other ways. Therefore, identifying the actual benefits of analogy-based simulations is an open research question. However, we posit that analogy-based simulations could have a number of advantages over unsimulated analogies, at least for certain use cases.

First of all, since they are interactive and dynamic, analogy-based simulations are likely to be more engaging to students than static, non-interactive presentations of analogies. Since students cannot benefit from an analogy if they do not engage with it, simulations may offer an advantage here.

A further potential advantage of analogy-based simulations is that they may help to address student misconceptions involving the analogy's base, target or both. Although students may be familiar with a system used as base, they may still hold misconceptions about it (*1*), which is likely to result in "mismapping" or "failure to map" features of the base to features of the target (*34*). While a student's misconceptions may be left unchallenged by an analogy involving images and text, the fact that a simulated system behaves according to actual physical principles, and not the student's imagination, means that students may recognize situations in which their intuition conflicts with the simulation. This could offer the possibility of conceptual change (*35*) and improved analogical mapping.

Additionally, a number of authors have described mental models of phenomena and processes as *runnable* (*36*) or involving mental simulation (*37*, *38*). This implies that many mental models are essentially simulations performed in a person's imagination. It is reasonable to expect that the use of dynamic simulations in instruction could aid students in developing more accurate mental models, which would be useful in future qualitative reasoning and problem solving tasks.

Finally, while analogy-based simulations may offer some benefits for most types of instructional content, we anticipate that analogy-based simulations could be particularly powerful in situations involving dynamic phenomena, especially those involving emergence. Emergent phenomena are typically very difficult for students to grasp, and though they may think they understand a particular system used as a base, they are likely to have misconceptions around any emergent behavior the system may exhibit (*39*, *40*). By providing them with highly constrained dynamic visualizations of physical systems, students may more fully confront misconceptions about emergent, dynamic phenomena than they would if systems were presented via text or static images.

As stated earlier, the actual benefits of analogy-based simulations are still to be determined. In addition, there exists the potential for drawbacks as well as benefits. We expect that any pitfalls of analogy-based simulations would align closely with the documented problems in using unsimulated analogies, which are described later, in the section on creating analogies.

In What Ways Can Analogy-Based Simulations Be Used?

There are two overarching scenarios in which analogy-based simulations may be used. The first involves using analogies to simulate concepts which are not possible or not feasible to simulate directly with depictions of atoms or molecules, or which could be simulated more clearly by analogy. A good example of such a concept is entropy. As a consequence, many curricula use analogies involving dice (*41*) or other simple systems (*42*) to discuss state degeneracy and, by extension, entropy.

The simulation in Figure 1 is another example of a concept that can be treated effectively using analogy. Though it is possible to create simulations of chemical systems that exhibit the Boltzmann distribution, students are likely to find simulations based on familiar, everyday objects more accessible and easier to reason about.

The second scenario in which analogy-based simulations can be used is focused on helping students to understand important abstractions that are used by experts in the domain. Abstractions and how they can be addressed by analogy-based simulations is the topic of the next section.

The "What" and "Why" of Abstractions

To this point, we have focused on analogies and the use of familiar physical systems to represent chemical systems by analogy. While analogy-based simulations can be used in a number of ways, one particularly powerful mode of usage is in helping students understand abstractions. In this section, we will discuss what abstractions are, why they are valuable, and how they can be conveyed to students.

What Are Abstractions?

In Gentner's seminal paper on analogy (*20*), she describes a related type of comparison that she calls *abstraction*. In her description, abstraction differs from analogy in that one of the compared entities is an "abstract relational structure" (*20*) rather than a concrete physical object or system of objects. An example of this type of comparison is the statement, "the solar system is a central force system" (*43*). Here, a concrete system of objects (the solar system) is compared to a central force system, which is an abstract relational structure commonly used in physics.

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In what follows, our interest is primarily in the abstract relational structure itself, rather than the comparison between it and a concrete system. As a consequence, we will shift our usage of the term "abstraction", from denoting the comparison described above to denoting the abstract relational structure itself.

As discussed earlier, systems can be modeled as consisting of a set of nodes, which represent components of the system, and internodal connections, which represent relationships between components. An abstraction can be thought of as that network of internodal connections, but without actual, concrete components at the nodes. That is, while the relationships between components are specified, at least in general terms, the components themselves are not. This enables the abstraction to act as a template for many different systems.

For example, a central force system possesses a central object, which is surrounded by one or more other objects that 1) are less massive, 2) revolve around it, 3) attract it, and 4) are attracted by it. From this definition, it can be seen that atoms also qualify as central force systems. Thus, because of its generality, instances (that is, concrete examples) of a central force system can exist on hugely different length scales (atom, solar system) and involve very different objects (sub-atomic particles, planets). Even the nature of the force (electrostatic, gravitational, etc.) is not specified.

The generality and flexibility of such abstractions enables domain experts to draw powerful connections between seemingly unrelated systems and lays the groundwork for expert organization of knowledge, as outlined in the next section.

Why Focus on Abstractions?

Beginning in the 1960's psychologists began to wonder what differentiated experts in a particular domain from novices. This curiosity led to many fascinating and useful discoveries. While there are a number of interesting results, for our purposes in this chapter, the key result is that experts' "knowledge is not simply a list of facts and formulas that are relevant to their domain; instead their knowledge is organized around core concepts or 'big ideas' that guide their thinking about their domains" (*44*). Glaser and Chi (*45*) elaborate on this by noting that "[e]xperts see and represent a problem in their domain at a deeper (more principled) level than novices."

The fact that experts understand their domain in a deeper, more abstract way than novices has been demonstrated across different domains in a number of studies in which experts and novices were asked to organize problems or representations into categories of their own invention (*46–48*). In each of these studies, in physics, computer science, and chemistry, respectively, experts were found to create categories on the basis of more abstract, overarching principles that govern the domain, while novices were found to choose categories mainly based on surface features.

Since education concerns itself with turning novices into experts, it is important to consider how we may help this process along with our students. In particular, in light of the above discussion, we may ask how we can help our students to develop domain knowledge that is structured like that of an expert.

Naturally, a person cannot be an expert without a breadth of domain-specific propositional and procedural knowledge, which traditional instruction provides. Furthermore, people can become experts by means of an education focused only on communicating propositional and procedural knowledge. However, this is a lengthy and arduous path, involving exposure to many, many examples and only gradual recognition of their hidden commonalities. A possible means to accelerate this process is to attempt to directly teach students the abstractions around which experts organize their domain-specific knowledge. Though understanding the core abstractions in a domain is not the same as expertise, it is a useful first step toward expertise and the knowledge structures characteristic of experts. Thus, we will focus on how we can use analogy-based simulations to help students understand abstractions.

How Can Abstractions Be Conveyed?

Now that we have established the potential value of abstractions, it is natural to ask how they might be conveyed to students. As discussed earlier, one approach is to compare a concrete system directly to an abstraction of which it is an instance. Like most everything, abstractions can be very difficult to understand if discussed in only general terms. By providing specific systems that are instances of the abstraction, and by explicitly mapping features of the instance to features of the abstraction, instructors are likely to help students to develop a clearer understanding of the abstraction.

However, while abstractions can be understood through direct comparison to a concrete system, they can also be understood as the "superordinate concept" (*49*) of which two concrete systems, compared via analogy, are both instances. For example, while the flow of electricity is notoriously difficult for students to understand, they are generally familiar with the way that water flows. As a consequence, in order to help students understand electrical circuits, analogous water circuits are often employed (*50*). In this analogy, flowing water corresponds to flowing electricity, water pressure corresponds to electrical voltage, a pump corresponds to a battery, etc. Glynn (*11*) notes that in this analogy, the superordinate concept is a circuit – an abstraction that applies to many specific instances of circuits, including electric, hydraulic, magnetic, and pneumatic circuits. Examining the correspondences between analogous systems permits identification of the key parts of the abstraction. From these analogous systems we can infer that a circuit consists of something that flows (water, electricity) through some conduit (pipe, wire) in response to some driving force (pressure, voltage) that is applied by some component of the system (pump, battery).

In our view, the direct comparison approach is best for introducing the abstraction, while setting up the abstraction as the superordinate concept between two analogous systems is best suited for deepening students' understanding of a previously introduced abstraction.

While we have used canonical examples from physics in the preceding discussion, there are numerous important examples from chemistry. In what follows, we will discuss chemical abstractions including thermally activated processes, entropy-driven processes, and a two-dimensional energy landscape

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diagram commonly used by experts in reasoning about thermodynamics and kinetics.

Creating Analogy-Based Simulations: Some Considerations

Now that we have explained the potential utility of analogy-based simulations and the value of abstractions, we can turn our attention to the question of how we may design analogy-based simulations to convey abstractions. The guidelines we present are a mixture of ideas gleaned from our own experience, as well as relevant guidelines drawn from the literature. Like those whose guidelines we cite, we must emphasize that these guidelines are preliminary and need experimental verification. However, they represent a good starting point for efforts in this area.

Of course, before we can make an analogy-based simulation, we first need an analogy to use. Creating an analogy can be a tricky process and is arguably more like an art than a science. However, below, we present some guidelines for creating an analogy that can form the basis of an analogy-based simulation.

Appropriateness of Chosen Target

As discussed earlier, each analogy consists of two concepts being compared: a familiar one, called the *base*, and an unfamiliar one, called the *target*. If an instructor already has a target in mind, it may seem as though we can immediately move on to choosing a base. However, before attempting to construct an analogy for the chosen target, it is worth considering whether using an analogy to teach the target is a suitable approach.

Else et al. (*14*) suggest that analogies be "reserved for important or abstract concepts and concepts that are prerequisites to further learning." This is because processing an analogy can be time-consuming (*51*) and cognitively demanding for students. Furthermore, it is well-documented (*1*, *7*) that analogies can give rise to misconceptions among students who attempt to carry the analogy too far. Therefore, before choosing analogy as the means to teach a particular target, consider whether the potential upsides of analogies, described earlier, outweigh the possible drawbacks.

If the chosen target is well-suited to treatment by analogy, the next step involves deciding precisely which features of the target should be addressed. Many concepts in chemistry are complex and nuanced. However, for students in high school and most undergraduate courses, addressing all of the complexity and nuance related to a particular concept is unnecessary and unwise. Therefore, the main features that should be addressed need to be identified and the other, more subtle features may be ignored. By simplifying the target, the job of choosing an appropriate base becomes much easier. Furthermore, simplifying the target permits the analogy to be simpler, which appears to aid comprehension (*34*).

In our work (*52–54*), we identified the energy landscape (*55–57*) (or potential energy surface), thermally activated processes, and entropy-driven processes as good candidates for treatment via analogy because of their importance across a number of science and engineering domains, as well as their abstract nature, which makes them difficult to understand directly. While the energy landscape of most systems of chemical interest is of extremely high dimensionality, when only one particular transition on the landscape is considered, it can generally be simplified to two dimensions, as depicted in Figure 2. We focused on this simplified two-dimensional representation because it is widely used by experts as a tool for problem solving and explanations.

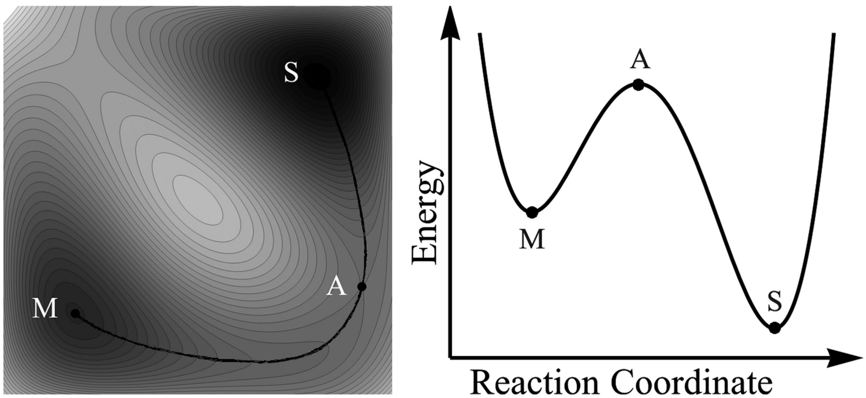

Figure 2. A very simple energy landscape represented as a contour plot (left), along with a schematic two-dimensional energy landscape diagram (right), which is a representation of the system energy along the reaction pathway, depicted as a black curve in the contour plot at left.

While powerful, this abstract representation of the energy landscape presents a number of difficulties for students. First, in some cases the y-axis represents potential energy, while, in others, it represents Gibbs free energy. The x-axis represents an abstract quantity called the *reaction coordinate*, which is created by abstracting the large number of system parameters involved in an actual, high dimensionality energy landscape down to a single variable. Understanding this axis alone represents a significant challenge for novices. Finally, the temperature is not represented in this representation at all. These three issues taken together make the representation of the energy landscape commonly used by experts very difficult for novices to interpret or use for reasoning qualitatively.

Choosing a Base

Once the target has been established, the next step in creating the analogy is choosing the base. The overriding concern at this stage is that the base and the target possesses *structural parallelism,* which Gentner and Holyoak (*58*) describe

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as "consistent, one-to-one correspondences between mapped elements". That is, in order for students to understand the key features of the target, there must be a clear correspondence between them and features of the base. This can be seen in Table I, where each important feature of the chemical system (the target) is "mapped" to a feature in the simulation (the base).

Beyond the requirement of structural parallelism, the literature contains a number of additional guidelines that should be taken into consideration when choosing a base. The most fundamental of these is that the base should already be *familiar* to students (*1*, *59*). Indeed, throughout this chapter, we have described the target as the unfamiliar part of the analogy, while the base is the familiar part. Without structural parallelism there is no analogy and without the base being familiar, the analogy is of little didactic value. So, these two requirements can be seen as the most fundamental when creating an analogy.

In the case that multiple potential bases are found that satisfy both structural parallelism and student familiarity, a number of additional selection criteria may be applied.

Harrison (*60*) found that using an *interesting* base can have a motivating effect on students, causing them to engage with the analogy. Conversely, a base that students found uninteresting caused students to lose focus and not engage with the analogy.

Work by Else et al. (*34*) suggests that simpler analogies, involving fewer mapped relationships, can be easier to understand. Unfortunately, the number of features that need to be mapped is largely a feature of the target and is not something that can be controlled solely through choice of base. In situations involving complex, multi-faceted targets, Spiro et al. (*61*) argue against the use of a single analogy, which is often oversimplified by students. Instead, they recommend an approach using multiple bases (multiple analogies). By choosing a number of analogies, each of which accurately captures a different aspect of the target, a better, more complete treatment of the target is possible.

Finally, for the purposes of creating an analogy-based simulation, it is necessary that the chosen base can be visualized in some way. Educational simulations are inherently visual, so, while a base that cannot be visualized could be of use in a textbook or in a lecture, such a base is inappropriate for a simulation.

In our work with the energy landscape we used a couple of different bases to illustrate the key relationships embodied by the abstraction of it that experts use. This abstract representational form involves a stable state, a metastable state, and an activated state, with the activated state (or energy barrier) lying in between the stable and metastable states. Thus, we needed to find a base that had features that could map to these states. The simplest and most familiar base we used for this was a cardboard box resting on a platform, depicted at bottom in Figure 3. In the curriculum that accompanied the simulations, we also provided 1,2 dichloroethylene as a simple example of a chemical system with states that qualitatively map to this energy landscape.

Figure 3 illustrates the fact that the box and 1,2 dichloroethylene could be used in an analogy as base and target, respectively, with the key relationships of the energy landscape captured by the analogy. Table II provides the mappings between the box and a general chemical system.

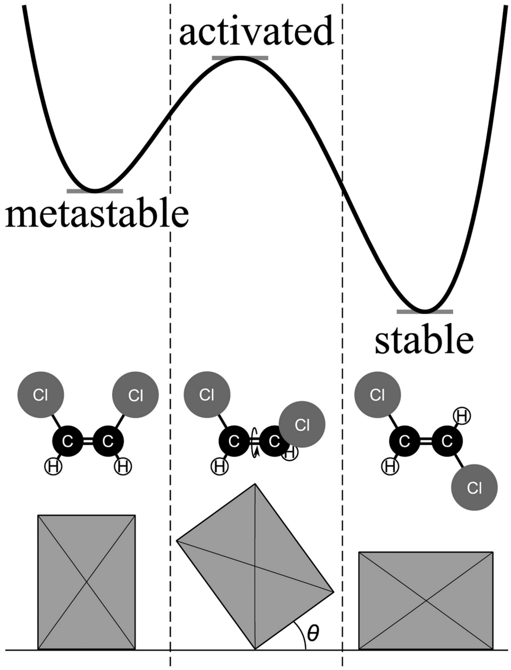

Figure 3. Correspondence of cardboard box and 1,2 dichloroethylene to the states in a schematic energy landscape.

Table II. Analogical correspondences between chemical system and box on platform system

Feature of Chemical System	*Representation in Box System*
State	Box orientation
Stable state	Box resting on longest face
Metastable state	Box standing on shortest face
Activated State	Box standing on corner
State energy	Box center of mass height
Reaction coordinate	Rotation angle

Considerations in Simulation Design

Once the target and the base have been chosen and the list of desired mappings is complete, we can move on to designing the simulation that will make use of the analogy. A number of authors have made suggestions for how to use analogies in educational texts or classroom settings (*10*, *12*, *31*, *49*, *62*). For our purposes, the key idea shared by these contributions is that the mapping between base and target must be made as clear as possible. While clarifying the mapping should be done

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in the curriculum that accompanies the simulation, the clarity of the mapping can also be enhanced through appropriate simulation design.

Since the goal of the simulation is to emphasize the correspondence between two different systems, providing visual representations of both systems simultaneously is crucial. Given this, we can turn to the literature on multiple external representations (MERs) (*63*) for some guidelines on how these simulations can be designed.

First, Ainsworth (*64*) recommends keeping the number of distinct representations as small as possible. Furthermore, each individual representation should not include too much information, lest it become too complicated for students to grasp. Tufte (*65*) also warns against the use of "chartjunk" – unnecessary graphical flourishes like gradients and other ornamentation, that can draw students' attention away from the actual informational content. From these guidelines, it is clear that we should strive for simplicity in our designs.

While simplicity is important, it is also imperative that students understand the features of each representation. In our work, in an effort to avoid cluttering the representations used in the simulation, we chose not to label everything in the simulation user interface. However, in order to ensure that students understood what everything represented, we provided labeled images of the simulation as part of the curriculum. We have also used "tool tips" to label items without cluttering the user interface. These are pop-up explanations or instructions that are visible only when a user positions the mouse pointer over a given user interface element. While these are two possible approaches, finding a good balance between simplicity and clarity may take some experimentation and testing with users.

In addition to considering the design of individual representations, we must consider how the connection between representations is conveyed. This can be done in a number of ways. Static approaches, such as using a single color to represent corresponding items across representations, can be helpful. Dynamic techniques, like "dyna-linking" (*64*), more fully couple the representations, such that a change in one representation produces a change in the other representation. While there are a number of techniques available to the designer, Ainsworth cautions against making the correspondences too obvious because this "may not encourage users to reflect upon the nature of the connection and could in turn lead learners to fail to construct the required deep understanding" (*64*). Here again, it is up to the designer to strike the appropriate balance, which is difficult to do without testing the software with users who are representative of the target population.

Putting It All Together

With these general guidelines explained, we will now discuss how to design a simulation based on the chosen approach for conveying the abstraction. Earlier, we discussed how we can address abstractions in two different ways. One way is to map a base directly to a target abstraction. The other way is to create an analogy between two systems that are both instances of the abstraction. In this approach, the analogy between the systems captures the important features of the

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abstraction. These two approaches to addressing abstractions suggest two different types of simulation, which we will discuss via examples from our work.

In the curriculum we designed, we chose the simplest examples we could find in order to first introduce the abstraction directly. Then, we used pairs of different systems to push students' understanding of the abstraction further. These two uses align with two of the three overarching categories of roles that multiple representations can play, as described by Ainsworth (*64*):*constraining interpretation* and *constructing deeper meaning*.

Constraining interpretation is very much like visual analogy and can be used to directly introduce abstractions. The idea is that by using one familiar representation and one unfamiliar representation, it is possible to help students to build an understanding of the unfamiliar via the constraints imposed by the familiar. In our work using the cardboard box as the base and energy landscape as target, we used dyna-linked representations of the box and its energy landscape as seen in Figure 4 to help students understand the connection between the box and its energy landscape.

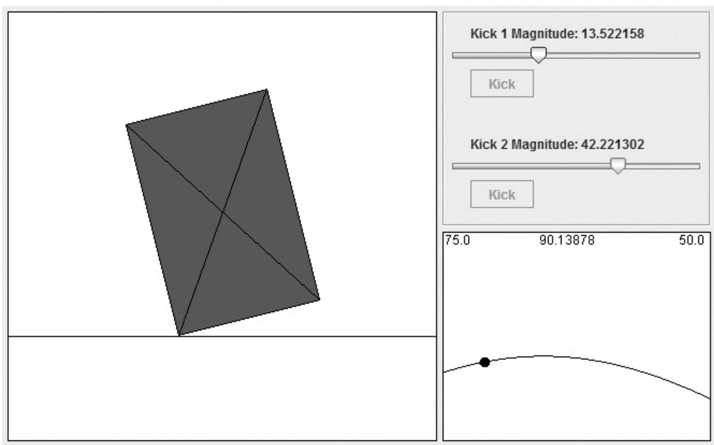

Figure 4. Visualization of a cardboard box on a platform along with a plot of its energy landscape, which is its potential energy as a function of rotation angle.

The goal of this simulation was to help students understand that a system can be in one of a few possible thermodynamic states, that those states each have a quantifiable energy, and that there is a transition pathway from one state to another. To help them grasp these ideas, students can "kick" the box and see how it responds. In the curriculum (*52*), they are asked to find the minimum kick magnitude that is sufficient to cause the box to transition from lying down (stable) to standing up (metastable) and vice versa. When the box is kicked, a dot moves on the energy landscape, showing how the box's current position maps to the energy landscape representation. Thus, using a familiar and accessible system, they may gain an understanding of the key attributes of the energy landscape: the activated state or energy barrier, which must be overcome when transitioning from one state

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to the other; the stable state, from which a larger kick is necessary to overcome the barrier; and the metastable state, which, by virtue of its higher energy, requires a smaller kick to cross the energy barrier.

In keeping with the guidelines introduced above, the representations of both the box and its energy landscape, as seen in Figure 4, are simple and clear. However, one representation-related issue that is not obvious from the figure is that the connection between the energy landscape and the cardboard box is only valid as long as the box remains in contact with the platform (*54*). If the box-as-base is to work, it cannot function exactly like a normal cardboard box, which could be kicked off the platform, into the air. Once the box leaves the platform, the analogy breaks and loses its didactic power. So, in this simulation, we had to add the constraint that the box remains in contact with the platform at all times. In the design of analogies or analogy-based simulations, it is important to watch for issues of this type.

Once an abstraction has been introduced, students' understanding of it can be extended by using multiple external representations to *construct deeper meaning*. In this usage, different systems that are both instances of the abstraction are set in analogy to one another. In a simulation, this involves presenting visualizations of these systems side-by-side. Giving students the opportunity to observe and compare superficially different systems that behave in similar ways can deepen students' understanding of the abstractions as "[l]earners can construct references across MERs that then expose the underlying structure of the domain represented" (*64*).

While we introduced the energy landscape with the cardboard box simulation, in order to deepen students' understanding, we needed an additional system with analogous behavior. We settled on a system involving balls bouncing on vibrating platforms, similar to the system in Figure 1. In this case however, the platforms map directly to states on the energy landscape, as seen in Figure 5.

Like Figure 1, this base was initially used to help students easily visualize and understand equilibrium state populations as a function of temperature. However, later in the curriculum, it was placed alongside a large group of cardboard boxes like the one in Figure 4, this time also on vibrating platforms, to demonstrate that, in spite of very different surface features, the two systems exhibit the same behavior, with equivalent populations of states at equivalent temperatures. The simulation, shown in Figure 6, creates an analogy between the two simulated systems and enables students to construct a deeper, more abstract understanding of the energy landscape that underlies both systems.

Finally, we should note that if the representations developed for use in a given analogy-based simulation faithfully capture the desired deep features, then those representations may be useful for related abstractions. The above representations were designed around the mappings in Tables I and II, where the focus is on state energies and populations. During the design process, however, we discovered that only small extensions were needed to use these representations to address the related abstraction of entropy-driven reactions, as seen in Figure 7.

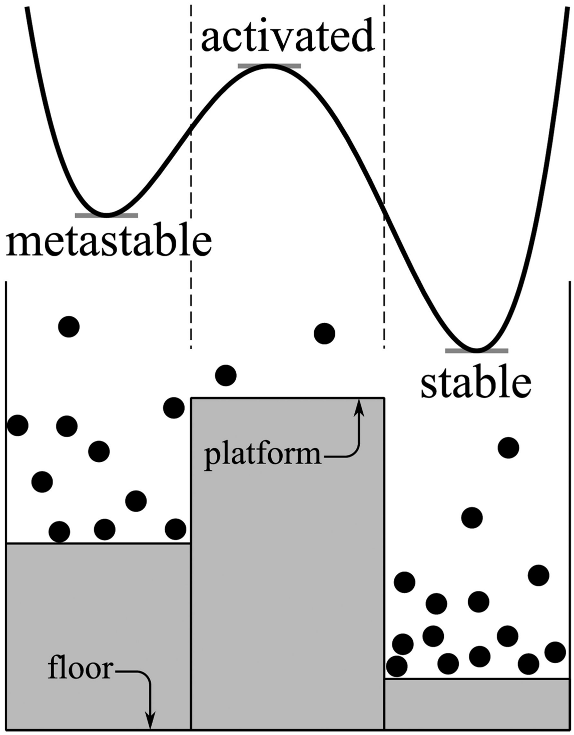

Figure 5. Analogical model of balls bouncing on a set of vibrating platforms and its correspondence to the energy landscape abstraction

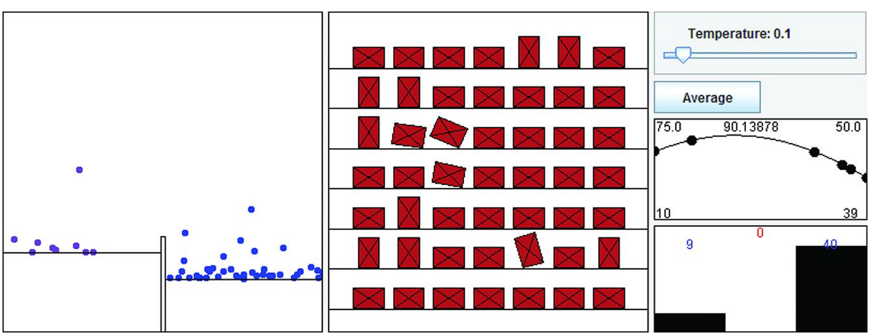

Figure 6. Two different bases set in analogy to one another in order to deepen understanding of the energy landscape (see color insert)

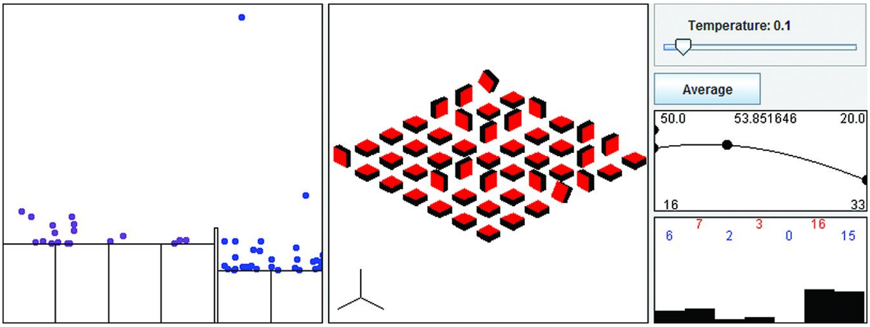

Figure 7. Three-dimensional boxes and balls bouncing on platforms corresponding to the boxes' faces. (see color insert)

In the platform representation on the left of Figure 7, a number of microstates (individual platforms) can be grouped into a single macroscopic thermodynamic state (the set of platforms with a given height). The number of platforms is the degeneracy of the thermodynamic state. In the three-dimensional box representation, the degeneracy of the states corresponds to the number of faces on which the box can rest with a given gravitational potential energy. Each box in Figure 7 has four ways to stand up and two ways to lie down. Thus, although the stable state is energetically favored, the metastable state's greater degeneracy makes it entropically favored.

In the platform representation, it is especially clear why the four higher-energy states have a higher population than the two lower-energy states at high temperature. This can then be mapped over to the box representation. These representations expose the key qualitative aspects of an entropy-driven process, illustrating that, at low temperature, low energy states are favored while, at high temperature, high entropy states are favored. These representations also motivate the use of free energy in chemistry, by showing how the population between two states is influenced by both the energy difference and the degeneracy (entropy) difference.

In this section, we have seen two different approaches to conveying abstractions by means of analogy-based simulations. In Figure 4, we presented a simulation that maps a simple, accessible base directly to a target abstraction and uses the familiar representation of a cardboard box to *constrain the interpretation* of the energy landscape representation. In Figure 6 and Figure 7, we presented simulations that create analogies between two systems with different surface features but common deep features in order to *deepen understanding* of the overarching abstractions. While much more could be said about software design, the design of effective educational representations, and so on, we hope that the guidelines and examples presented here will be a helpful starting point for individuals interested in developing similar materials.

Conclusion

We have presented a brief overview of analogy and how analogy can be used as the basis for simulations. In addition, we have examined abstractions, why they are valuable, and the manners in which they may be conveyed to students. We then merged that information with information on the use of analogies and multiple external representations to present guidelines on how analogy-based simulations may be designed in order to help students understand abstractions. We hope this contribution will help other researchers to join us in developing and testing analogy-based simulations in order to advance our understanding of how they may be effectively used to help students grasp both abstractions and other difficult and abstract concepts.

Finally, we would like to take the opportunity to stress that we are not arguing for the replacement of simulations involving direct depictions of atoms with analogy-based simulations. Neither are we advocating that traditional, detail-oriented instruction be replaced with a focus on abstractions. Rather, we are arguing for the use of abstraction-focused analogy-based simulations as a *complement* to traditional approaches. We feel that simulations like those described in this chapter have the potential to help students synthesize what they learn during normal instruction into well-organized groupings, setting them on a path toward expertise.

Acknowledgments

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57. In this chapter, we sometimes refer to the energy landscape as an abstraction. However, every chemical system has an energy landscape – a function that specifies its potential energy in terms of all relevant system parameters. In this sense, a system's energy landscape is not an abstraction; it is simply a complex attribute of the system. However, among experts, two dimensional energy landscape diagrams are used to represent as qualitatively similar many systems that do not possess even remotely similar sets of relevant system parameters. By examining these qualitatively similar diagrams, we see that, in fact, the two dimensional energy landscape drawn by experts is an abstract relational structure, possessing three states in specific relationship to one another: a low energy stable state, a medium energy metastable state, and a high energy activated state situated between the stable and metastable states. Therefore, though a system's energy landscape itself is not an abstraction, the representation of it used by experts is.
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Chapter 16

Teaching Tools for Organic and Bio-Organic Chemistry

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There are many tools that instructors of organic chemistry or biochemistry can use to enhance their students understanding of the material. Some learning tools improve learning by presenting new information (e.g. texts), some tools are beneficial because they involve senses that are otherwise uninvolved (e.g. model sets and 3D visualizations), and some tools are useful because they give students additional time on the subject (e.g. textbook problems and online homework). In this chapter we will summarize the various tools that are available for organic chemistry and biochemistry. In particular, we will review five software packages that have provided useful visualizations for the molecular events that occur in organic chemistry and five online products for helping students visualize the bio-organic molecules that are discussed in a typical biochemistry course.

We have seen, in the previous chapters in this compilation, that students benefit from well designed visualizations. We also know that learning is enhanced by visualizations. The improved understanding that results from well-designed learning tools is often simply a result of increased time on task. But some students have a difficult time visualizing certain objects, such as molecules. For those students visualizations bring a deeper understanding of the three-dimensional nature of Nature.

In this chapter we will address specific software packages that are available for students in organic chemistry and in biochemistry. Hopefully this survey of

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ACS Symposium Series; American Chemical Society: Washington, DC, 2013.

the available tools will be helpful to instructors and students. It is my hope that the survey will also be thorough. But I am a realist and I expect that in my search I have missed some of the available software packages out there. A subsequent paper may be necessary, in order to capture a more complete list of software as a result of input from readers.

Part I. Teaching Tools

There are many valuable resources for instructors and students striving to teach and learn organic chemistry. First, and in my opinion foremost, is the textbook. There is no substitute for reading a well-written informative text. This must be a general opinion; there is no shortage of options for organic or biochemistry texts. For example, one can find at least 15 Organic Chemistry texts on the market and, partly because of the competition, each one has its attributes (*1*). While there are fewer biochemistry texts (*2*), the significant challenge of covering the entire topic of biochemistry makes the textbook essential.

A second resource is the electronic version of the textbook. The demand for electronic resources has increased in the past 10 years, so most of the recent texts are now available as ebooks. Students still prefer the hard copy (*3*), but it is likely that the demand for electronic texts will increase with time.

An important resource for molecular sciences is the model set. Model sets have been useful chemistry teaching tools for at least 50 years. Perhaps the first accurate molecular model kit that was available for student use was produced by C. Arnold Beevers, who was a crystallographer at the University of Edinburgh. His model sets were made available in 1961 (*4*). The ability to make plastic molds was necessary for the mass production of the Beevers Miniature Models as well as the many student-oriented kits developed since 1961.

Those who teach organic chemistry often require their students to obtain a model set. Students benefit from the tactile interaction with models of atoms and bonds (*5*). Although there is some inaccuracy in the representation, having a stick represent a bond and a ball represent an atom allows the student to assimilate valuable molecular information. The macromolecular nature of biochemistry does not lend itself well to the use of model sets. But a few model sets for biological macromolecules, such as DNA, have probably been more useful as a learning resource than any other tool. A history of the model sets for large biomolecules has been compiled by Martz and Francoeur (*6*).

Finally, visualizations have been a resource for learning chemistry since textbooks began including drawings (*7*). For organic chemistry and biochemistry, the necessity of drawings can not be overstated. They are "indispensible tools for presenting evidence" (*8*). Textbook figures aren't the only way students can comprehend molecular images. Other methods for visualization include computer rendered structures, including molecules that can be manipulated by the user. The computer rendered image as a visualization tool is the subject of this chapter.

Part II. Organic Chemistry Visualization Tools

Visualization tools include drawings, simulations, and animations. The drawings that are provided in organic chemistry texts have made dramatic improvement over the years. The first widely used American organic textbook was written by Ira Remsen and published in 1885 (*9*). There were several German texts on the subject by that time (for example: Carl Lowig, 1853; V. v. Richter, 1876; and Adolf Pinner, 1876), and the structures drawn in those original German works were impressively accurate and clear. Interestingly, the English translated versions of the same texts were less definitive in their representation of the structures.

Perhaps more than any other field, organic chemists benefit from modern printing technology. The use of improved three-dimensional perspective and color in the drawing of structures has illuminated organic chemistry to the most comprehensible level (Fig. 1).

(a) (b) (c)

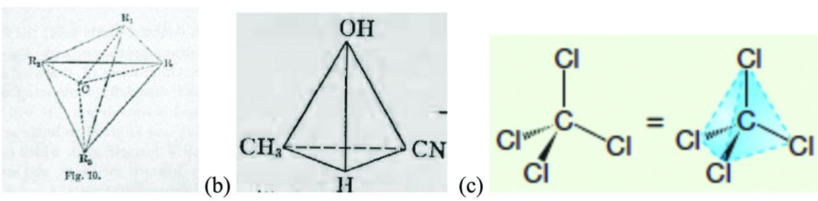

Figure 1. Three eras of organic drawings: (a) Ira Remsen, 1889, p. 164; (b) Louis Fieser and Mary P. Fieser, 1944, p. 263; (c) Maitland Jones, Jr. and Steven A. Fleming, "Organic Chemistry" W.W. Norton, 2010, p. 52. Reproduced with permission from W.W. Norton.

There are computer rendered step-wise representations that allow the student to visualize changes in molecular structure from one point to the next. I will not classify the use of these still-images as animations. They are slides that show a structure, and the user can move from one to the next visual representation (*10*). A student can use this type of teaching tool to repeat a classroom presentation, for example. This teaching tool also lends itself well to use by an instructor who uses powerpoint type presentations for the classroom.

A teaching tool that provides three-dimensional perspective can help students who are challenged by depth perception (*11*). For example, it has been difficult to give students a real appreciation for the inversion that occurs in the S_N2 reaction. Textbook figures have sufficed for teaching generations of organic chemists about this particular reaction. However, in spite of the excellent textbook representations and the use of umbrellas in the classroom, we know that some students still struggle with the concept of inversion. Model sets aren't much help on this particular reaction. The author is unaware of any commercially available sets that have rehybridizable atoms, which would be necessary for the inversion process. On the other hand, a computer animation using xyz coordinates (i.e. 3D) is an excellent method for illustrating the process.

Computer animations also have the advantage of student access in a classroom, a laboratory, or at a time outside of class. The images are viewed on a computer screen and therefore technically two-dimensional. However, advanced software packages are available that add shading and appropriate size modification as objects move from background to foreground. The observer is able to visualize the images as 3D, just as we can see a train coming on the silverscreen. There are several software programs that have been used for this purpose.

Another way to experience the 3D perspective is for the student to have the ability to change her viewing angle of the image. One can appreciate the overall process in the animation from a variety of perspectives in order to add depth to the understanding. There are very few organic chemistry events that involve 3-4 atoms, which means that multiple angles of viewing can help the user catch all the details.

There are other important features of a good teaching tool. The ability to zoom in or zoom out is useful. Having different background setting options can help for viewing. Pausing and restarting an animation is a desirable option. This is particularly true if the animation has multiple moving atoms. Comparison of the animation with a textbook figure within the animation helps the student connect the two resources.

I have chosen five programs that provide animations for students learning organic chemistry. Undoubtedly there are other programs that have been produced. My choices are based on historical significance and level of accuracy of the animations.

1. Organic Reaction Mechanisms

The first animation software for organic chemistry that involved reactions was probably “Organic Reaction Mechanisms” by Andrew Montana and Jeffrey Buell from California State-Fullerton. This software was novel at the time of its release. It was commercially available in 1996. It had animations of more than 60 reactions. Most of the reactions had an accompanying energy diagram. Professor Montana added orbitals for some of the reactions. The molecular motion was not particular smooth, but the idea was new for 1990’s. Prof. Montana received the Merlot Award in 2006, although it was for a teaching tool indirectly related to Organic Reaction Mechanisms (ORM). The publishing company for ORM was Falcon Software (Wellesley, MA); unfortunately that company no longer exists, and Dr. Montana passed away in 2007.

The most recent version that I could find lists a compatibility with Mac OS 7 and Windows 3.1, which suggests that it isn’t likely to run on today’s operating systems. In spite of our inability to use the software today, the initial product was a giant step forward in the field of animating organic chemistry.

Program Attributes

The software provided the textbook version of the reaction on the page that ran the animation. The student could stop the animation and restart it. The program displayed an energy diagram associated with the animated process for several of the reactions.

Improvements

The hand-drawn structures were not completely accurate models, particularly the orbitals that were drawn for several of the reactions. The data used for the animation was not from an xyz file. That is, the animations weren't cleanly represented in three dimensions. That also meant, of course, that the student could not manipulate the viewing angle.

Although there were limitations to this original program, its contribution was significant. It was the first demonstration of the power of enhanced learning of organic reactions by using the computer.

Sheri Strickland at Converse College in Spartanberg, South Carolina has a new animation package for organic chemistry (*12*). Her software, which currently only works on a PC, can be found at: http://cs.converse.edu/~phbrown/OrbitalVis. This teaching tool is similar to Montana's Organic Reaction Mechanisms. It is a useful resource for students to access online.

2. Organic Reaction Animations

Development of Organic Reaction Animations (ORA) began in late 1996. I became aware of Montana's ORM software (see above) in early 1996 because fellow chemist, Ty Redd (*13*), brought it to my attention. My colleague at Brigham Young University, Paul Savage, suggested that we use calculations to improve the ORM visualization tool and more accurately represent the reaction pathways. We submitted our first proposal for funding of the software development in October of 1996. In what proved to be the best decision for the future of the ORA software, we brought undergraduate Greg Hart into the project. Greg was familiar with state-of-the art computer animation software at that time, and he is also a very talented computer graphics designer. He coordinated the team of animators (*14*) that created the animations over the next several years.

Paul Savage and I presented our first version of ORA at the ACS Fall Meeting in Las Vegas in 1997 (*15*). It had about 20 reactions at that point in time. It was as a result of that ACS presentation that the publishing company W. W. Norton became involved in the project. One of the unique aspects of ORA is that the user can view accurately represented molecular orbitals for each reaction. ORA uses Frontier Molecular Orbital theory to demonstrate the nucleophile reacting with the electrophile, which is a common theme of all organic chemistry. It's also a common theme in the text "Organic Chemistry" by Maitland Jones (published by W. W. Norton), so our product had a natural fit with the Jones text.

The first marketed version of ORA was produced in 1998 with about 30 reactions. The number of reactions included in the software continued to grow until it reached 52 reactions in the version released in 2000. ORA has been upgraded several times since 2000 due to changes in Mac and PC operating systems, and it has been wrapped with the Jones text and sold separately by W. W. Norton continuously since 1998.

Creation of the reaction animations in ORA was accomplished by the following process (*16*). First, the reaction was modeled using Spartan (*17*) software. The semiempirical (AM1) calculations provided an accurate xyz file for the animation. Several points along the reaction path were calculated, in order to show the atom locations and the orbital shapes throughout the process (Fig. 2). Calculations along the reaction path were obtained by putting minimal constraints on interatomic distances between the nucleophile and the electrophile and performing energy minimizations. Each reaction had 20-50 calculated points.

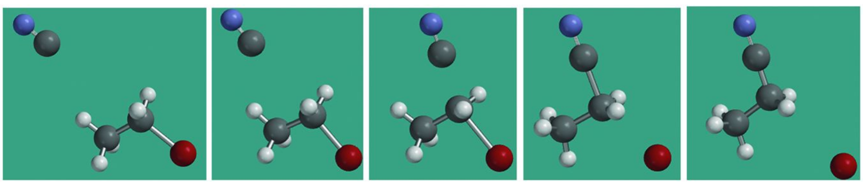

Figure 2. Step-by-step calculations of an S_N2 reaction.

The second step required translating the xyz files of Spartan into the 3D imaging software called Maya. It was the use of this 3D software that resulted in an improved view and better understanding of each reaction (*18*). In this step, the 20-50 calculations are melded so that a smooth process from the starting position to the end is obtained.

The final step has the Maya file for a given reaction put together with the timing on the appropriate energy diagram, and the matched pair are then converted into a Quicktime movie and placed into Director. The ORA user can select the reaction and observe it as a ball and stick, space-filling, or orbital animation (Fig. 3).

In 2001, Greg Hart helped us create an interactive version of ORA called Interactive Organic Reaction Animations (iORA). In order to produce this software, we needed a program that would allow for an animation to have the viewing angle changed during the animation. There were relatively few options at the time. We chose to use Cult3D for the interactive version of ORA. It worked well for 2 years, running on the PC platform, but it never ran on Mac; and Cycore, the company that produced Cult3D, ceased to support iORA in 2003.

In Pedagogic Roles of Animations and Simulations in Chemistry Courses; Suits, J., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2013.

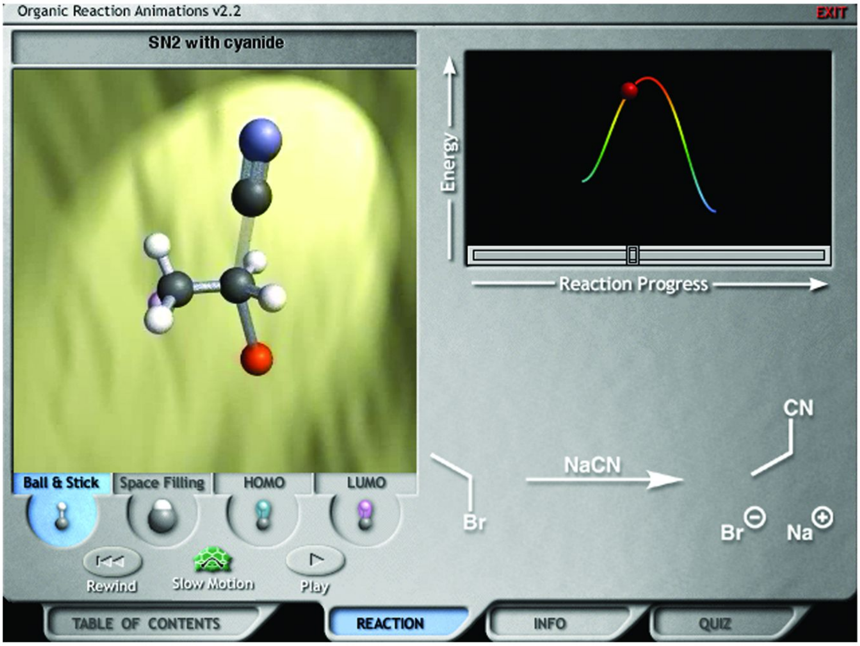

Figure 3. Screen shot of Organic Reaction Animations (19). Reproduced with permission from reference (19). Copyright 2006 W.W. Norton.

Program Attributes

Each reaction provides the textbook version of the reaction that can be viewed while the animation plays. The student can stop the animation and restart it and move the reaction to a particular point on its reaction pathway. The reaction pathway is shown as an energy diagram that has a marker showing the current position in the pathway throughout the animation. There is a quiz page that the student can use to test their understanding of the reaction. This can be done while the reaction is running. The software runs on PC platforms and on Mac platforms up to OS 10.6.8.

Improvements

Although iORA allowed the user to change the viewing angle, it is no longer supported. ORA does not allow user manipulation. The software only runs off of a CD (*20*). The software is not free.

In Pedagogic Roles of Animations and Simulations in Chemistry Courses; Suits, J., et al.;
ACS Symposium Series; American Chemical Society: Washington, DC, 2013.

3. ChemTube3D

Nick Greeves and Neil Berry at the University of Liverpool have developed a website called ChemTube3D. The project was initiated in 2007 and it has grown considerably since then. Numerous students have assisted in the development of the program (*21*). Support for the project has come from UK Physical Sciences Centre, JISC, and EPSRC. Inspiration for developing the teaching tool came from teaching stereoselective reactions such as the Diels-Alder, which required an appreciation of the spatial 3D arrangement of molecules as they react to explain the stereochemical outcome (*22*). The associated endo stereoselectivity continues to be one of the most visited pages on the website.

Creation of the organic animations in ChemTube3D was accomplished by first using Spartan (*17*) to calculate the transition state and then GAMESS (*23*) or Firefly to produce the xyz coordinates of a series of frames for the reaction process. The output files were transferred to MacMolPlt (*24*) in order to develop the whole animation. The animations are viewed and controlled in the website using Jmol (*25*). The program is available online at www.chemtube3d.com

Program Attributes

There are well over 70 reaction animations on ChemTube3D. Each animation provides the textbook version of the reaction that can be viewed while the animation plays. The user can choose a variation of the animation that shows the electron-pushing version of the process. The student can stop the animation and restart it and move the reaction to a particular point on its reaction pathway. Reaction pathways are calculated, so the representations are fairly accurate (Fig. 4). The user can manipulate the reaction as it is running. The software runs on Mac and PC platforms.

Improvements

Many of the reactions, perhaps half, are advanced level chemistry. That is, the typical service level organic chemistry course will not need to learn the Mitsunobu reaction, the S_N2' reaction, or nitrile oxide synthesis. Several of the reactions that are animated include multiple steps, however the reactions are animated by step so these multi-step reactions can only be viewed step-by-step. There is no way to view the complete process of acetal formation, for example. There are no orbitals shown in the animations. When new bonds are formed, the animation represents them initially as broken bonds rather than fading them in.

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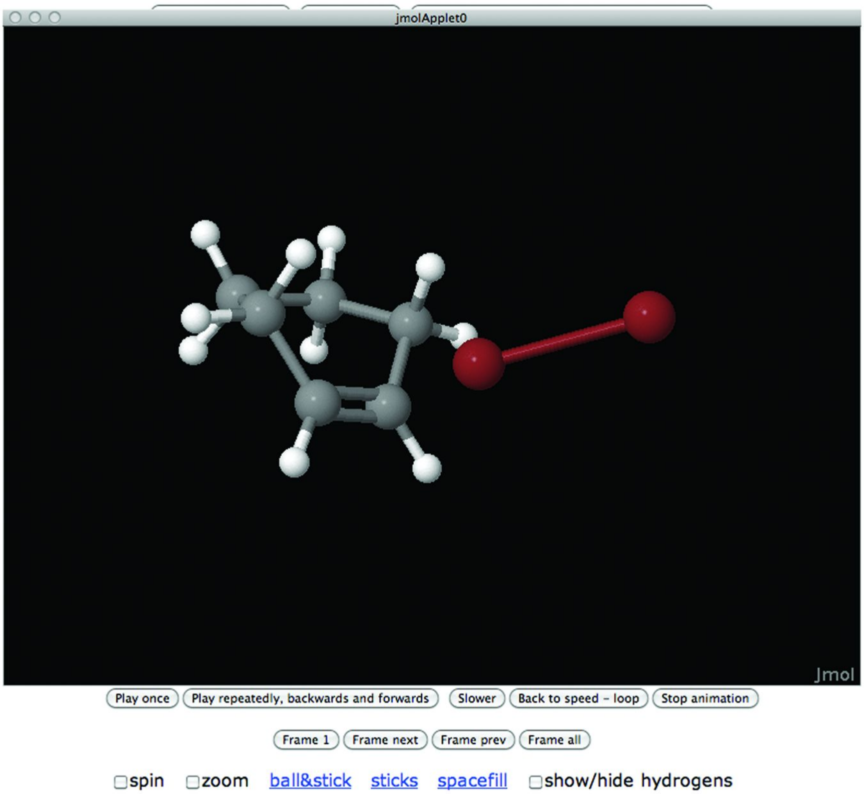

Figure 4. A screenshot of the bromination of cyclohexene ChemTube3D animation (26). Courtesy of Nick Greeves.

4. Spartan (*17*) (Wavefunction)

Wavefunction, Inc. was founded in 1991. The company markets the program Spartan, which is a computational package that allows researchers and educators to do high-level molecular modeling calculations. It is one of the most useful tools for organic chemists. In 2000 the Spartan program included an option for animating chemical events. Unlike the three software programs listed previously, the Spartan animations are not pre-designed. Once a student learns how to do the animations, she can design her own pathways. Although this is empowering, it is likely that most of the learning would occur prior to getting the animation to run. A student would need to work with the computer images of xyz files (3D data) in order to prepare a molecular sequence that shows the reaction of interest.

There are other commercial products that are comparable to Spartan. One such product is marketed by CAChe Research. The CAChe software program that can be used to produce animations for teaching purposes is MOPAC2012 (*27*).

Program Attributes

There is no limit to the number of animations that can be produced. The student can stop the animation and restart it and toggle the reaction forward or backward to a particular point on its reaction pathway. Reaction pathways are calculated, so the representations are fairly accurate (Fig. 5). The user can manipulate the reaction as it is running. The software runs on Mac and PC platforms.

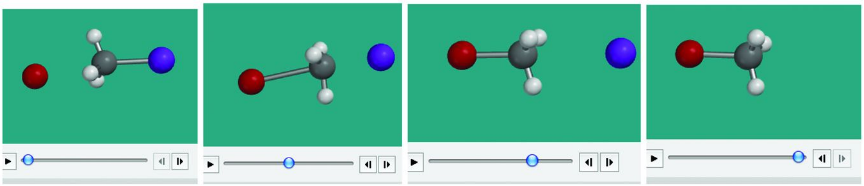

Figure 5. Using Spartan to demonstrate a chemical reaction.

Improvements

It is not possible to control the speed of the reaction animation, and the animation runs back and forth rather than in one direction. The presentation is not as clear as it could be. The multiple-step reaction would be very difficult to construct in a single animation using Spartan. The biggest obstacle to using this software as a teaching tool is the cost. The complete Spartan package is fairly expensive for large classrooms of users. Although the basic software is affordable for use by large groups, it is not clear that the animation option is included in that package. In terms of teaching tools, it is clear that Spartan is outstanding.

5. Mol4D

Hens Borkent at University of Nijmegen in the Netherlands produced an animated organic chemistry teaching tool that is web-based (*28*). The product is called Mol4D, and it comes from the Web Tutorials in Chemistry (WeTChe) project, which was sponsored by the University of Nijmegen Center for Molecular and BioInformatics (CMBI). Development of Mol4D was initiated in the early 1990's. The initial scriptwriter for the software was Jack Leunissen. The original tutorial nature of the program had students viewing molecules online in order to see the 3D perspective. MOPAC calculations are possible on-the-fly using this program; and the idea of putting together more than just bond rotations in the animations led to the inclusion of animated reactions. The original visualization used Chime for display of the animations. Recently, Jmol has been substituted as the viewing tool since, unlike Chime, it is compatible with PC and Mac platforms.

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Program Attributes

The learning opportunities are maximized in this unique software. No other teaching tool allows the student to interact as completely as this program does. The animations are not “canned,” which means that the student can propose her own choice of reagents. For example, the S_N2 reaction can be studied by varying the nature of the electrophilic alkyl halide. It is possible to compare calculated results for nucleophilic attack on methyl bromide, ethyl bromide, isopropyl bromide, and *t*-butyl bromide. The MOPAC calculations are displayed in 3D fashion that can be manipulated by the user. The data are also shown in graphical fashion, so the student can compare the calculated energy barriers (Fig. 6). This allows the students to discuss the results and draw conclusions based on their exploration.

Mol4D is available online at: http://wetche.cmbi.ru.nl/organic/indexe.html.

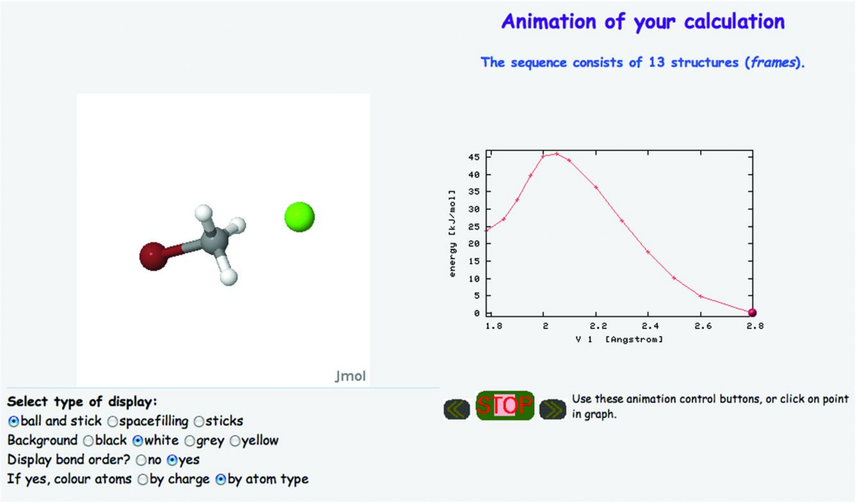

Figure 6. A screen shot of Mol4D (29). Courtesy of Hens Borkent.

Improvements

Unfortunately, Hens Borkent has retired and is no longer updating this program. The current version of the software is operable. There is a learning curve associated with using the tool; but once the user figures out the process, Mol4D opens the door to laboratory-type investigation.

Part III. Bio-Organic Visualization Tools

There are several reasons that teaching the chemistry associated with biochemistry requires good visualization tools. First, and most obvious, is that most of the biomolecules are simply too large to represent quickly on a chalkboard. Model sets are not as useful either; however, one can obtain a good model set of DNA.

A second reason for needing a good visualization tool is that 3D is so important to the topic of structure and function. It is difficult to gain an appreciation for the binding site of a particular enzyme by looking at a 2D picture in a textbook. The chemistry of enzymes, lipid membranes, nucleic acids, and carbohydrates is very dependent on the shape of these molecules.

Another important factor is the increase in the number of students taking the biochemistry courses. The medical schools are expecting students to have more understanding of biochemistry principles than was expected in the past. This will mean schools will be teaching larger sections and trying to reach more diverse learning styles, which is a natural result of having a larger class. There will be more demand on good teaching tools for helping students understand the principles associated with biomolecules.

I have chosen five programs that provide animations for students learning biochemistry. I am aware that there are other programs that have been produced. A quick search on the internet reveals many additional tools. The summary presented here is simply limited by time and space.

1. Bio-Organic Reaction Animations

Bio-organic Reaction Animations (BioORA) is a natural extension of the ORA software discussed above. The focus for BioORA is the molecular level of the chemistry that occurs in biomolecules. The teaching tool was developed so that students would be better able to visualize the structures involved in biochemistry and to reinforce the organic chemistry that is associated with several classes of reactions.

Development of the software was initiated in a collaboration with Greg Hart and Paul Savage in 2003 (*30*). More recently, I have been responsible for the content of the software; and the Brigham Young University Center for Teaching and Learning, most notably Robert Allen, has provided the software programming of BioORA.

This teaching tool has the following chapters: enzymes, carbohydrates, lipids, and nucleic acids. Each animation is based on a crystal structure obtained from the Protein Data Bank (pdb). There is a short description of the significance of the particular biomolecule and an animation showing the chemistry related to the structure (Fig. 7). References are provided that support or question the steps illustrated in the animation.

The animations are based on MM2 type calculations, since the complexity of the macromolecules—and the role that water must play—make higher-level calculations difficult and less meaningful.

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Program Attributes

One of the advantages of this software is that it covers more than just one topic, so an instructor can use the program to guide the students through a full semester of biochemistry. Another advantage is that the emphasis is on the molecular structure of the biomolecules. There are very few places where the atoms are hidden. This may not be an attribute that is appreciated by all students, because many instructors of biochemistry are inclined to use non-molecular representations of biomolecules (i.e. blobs, boxes, or acronyms).

The software gives the user the ability to rotate the 3D structures as the reactions are shown. There is an option of seeing the whole process animated or of watching the events in a stepwise fashion. The software has quiz questions associated with each animation and a textbook representation of the chemistry that is animated.

BioORA is free, accessible online, and the software is compatible with Mac and PC. It uses Jmol and JAVA for viewing the macromolecules and it has a user-friendly interface.

Improvements

A common complaint about the software is that the user really must concentrate to find the reactive groups. It would be helpful to have a mouse-over identification of amino acids, for example. Perhaps this will be possible in future upgrades of the software. It is possible to move between the ball and stick representations and the ribbon structures of the enzymes, but this switching is not particularly smooth.

BioORA is available at: www.ctlbyu.org/bioora.

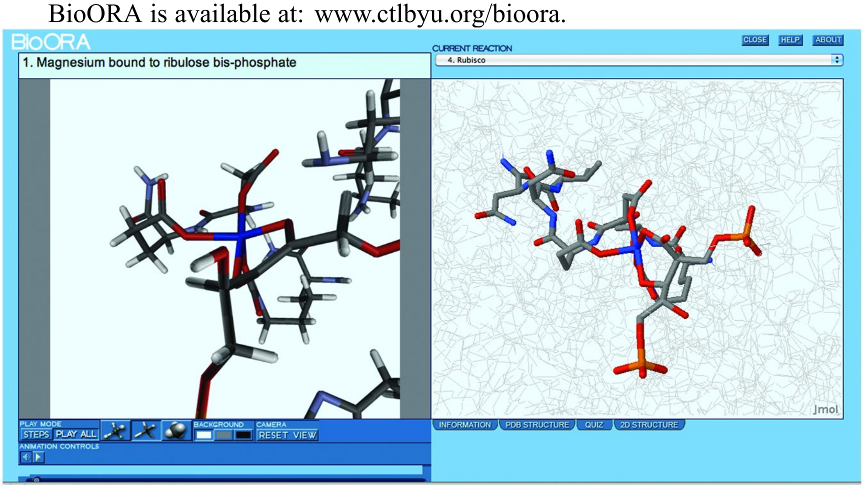

Figure 7. A BioORA screenshot of the rubisco enzyme. Reproduced with permission from BioORA. BioORA can be accessed at www.ctlbyu.org/bioora. (see color insert)

2. Individual Products

Shari and Stephen Dunham at Moravian College located in Bethlehem, PA have produced several models of amino acids and peptides. They use JAVA to illustrate small structures (Fig. 8) in 3D accurate images that are available on Shari's Blackboard site (*31*).

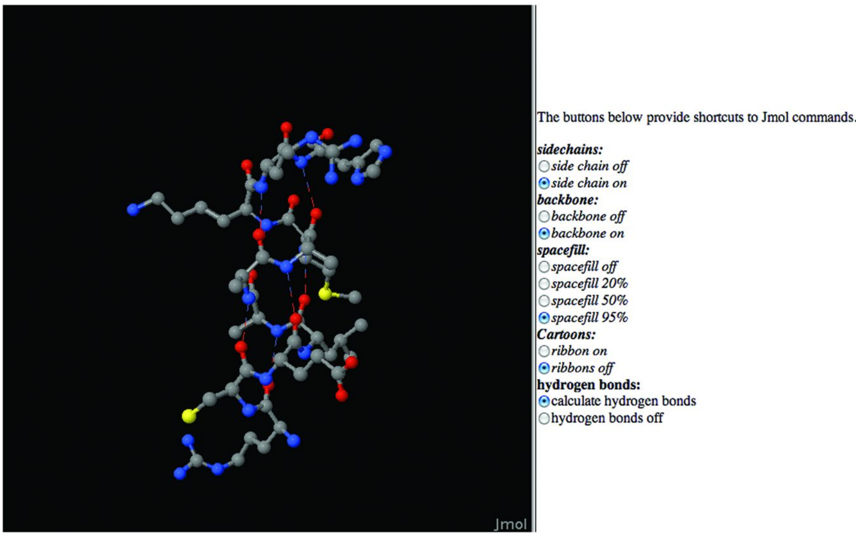

Figure 8. Calculated structure shown on Blackboard site created by Shari and Stephen Dunham. The user can manipulate the figure. Courtesy of Shari Dunham.

John Kyrk has produced animation of peptides that are drawn structures. These animations are useful for beginning biology students. The structures are only approximations, and the reactions are not based on standard organic chemistry mechanisms (Fig. 9). However, for students who have not had organic chemistry, or who have chosen to minimize their organic chemistry, the visualizations are probably useful. Perhaps the target audience is high school students. This software can be accessed at www.johnkyrk.com/aminoacid.html.

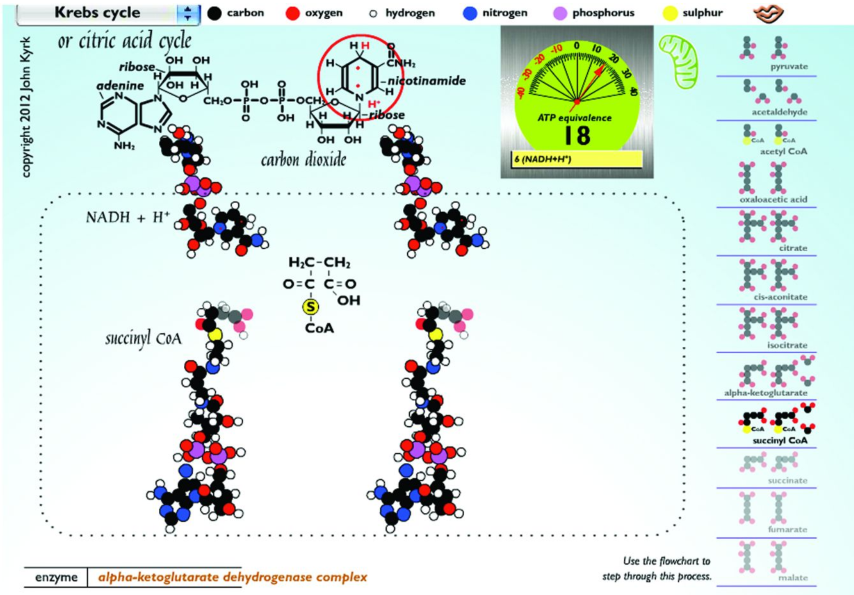

Figure 9. Cartoon drawings by John Kyrk (32). The user cannot manipulate the structures. Courtesy of John Kyrk.

3. BME3D

Eric Martz and Frieda Reichsman at University of Massachusetts have produced an excellent set of animations for use by biochemistry students. Angel Herraez contributed a significant portion of the biomolecule content, particularly the material under the "Carbohydrates," and that material appears to be directed at high school students. The original work used Chime as the visualizing software. Recently, BME3D was modified so that Jmol is used for viewing the 3D images. Eric Martz is responsible for the software of FirstGlance in Jmol. The animations are only rotations of the 3D images--there are no molecular motions shown. The structures are accurately represented, apparently energy minimized conformations. There are good references for the lipid membrane material.

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Program Attributes

BME3D is easy to use; and it has 3D images of proteins, carbohydrates, lipids, and nucleic acids. It also has a chapter on water and one on vitamins. The text is available in English and Spanish. Students are able to rotate the 3D structures using Jmol, and there's good use of color to help identify various moieties throughout the step-by-step presentation (Fig. 10).

BME3D is free, accessible online, and is compatible with Mac and PC platforms. It uses Jmol and JAVA for viewing the macromolecules, and it has a user-friendly interface.

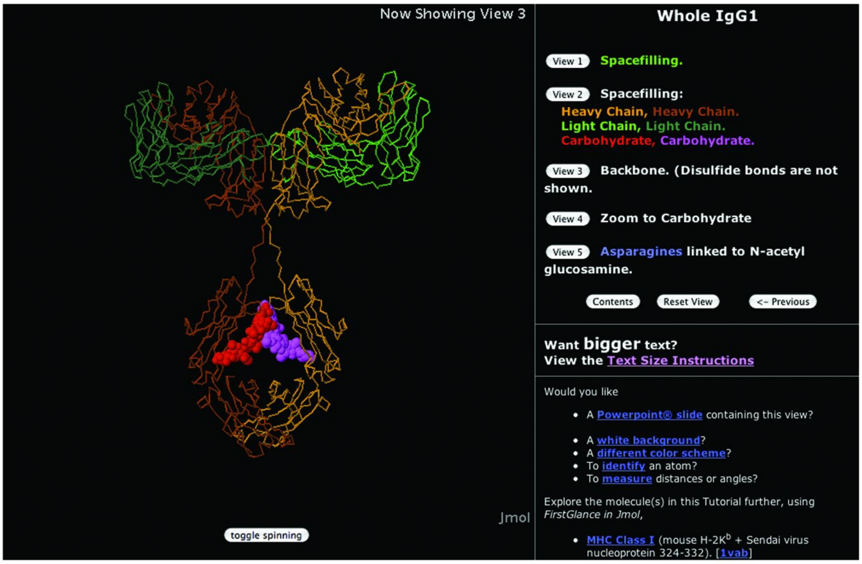

Figure 10. BME3D of antibody IgG1 (33). The user can manipulate the structure. Courtesy of Eric Martz. (see color insert)

Improvements

It is not clear which structures are taken from crystal data and which are calculated structures. There are some structures that are poorly represented (vitamin B_2, for example), but this is a minor issue. The software representation of double bonds and the excess use of color on some of the 3D images is non-ideal (see "Amino Acids" in the "Carbohydrates" heading).

BME3D is available at www.umass.edu/molvis/bme3d/.

4. Wiley Animations for Voet/Voet/Pratt

Publishing companies have been providing more supplements for their texts since the personal computer has become a significant tool in post-secondary

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schooling. Each of the biochemistry texts provides access to software that can enhance the learning experience. The Wiley animations are similar to many other static flipchart type presentations. The images are not calculated nor are they drawn with any 3D perspective. These "animations" are powerpoint slides that give students another opportunity to view the material.

Program Attributes

The Wiley product is easy to use and provides a connection between the visualization and the Voet and Voet textbook. Each chapter has several selections that allow for extra time on task. Access to the slides is free.

Improvements

Perhaps this product shouldn't be included in the comparison provided in this paper. There is very little that is animated, and it is not shown with any intent to be accurate. Reactions are drawn without showing the reactive intermediates, and there is no biological chemistry in the presentations. For example, the rubisco enzyme that is involved in the conversion of ribulose-1,5-bisphosphate into two molecules of 3-phosphoglycerate has magnesium coordination, which plays an important role in the hydration step of the ketone shown in Figure 11. The magnesium coordination is not shown in this page of the slideshow.

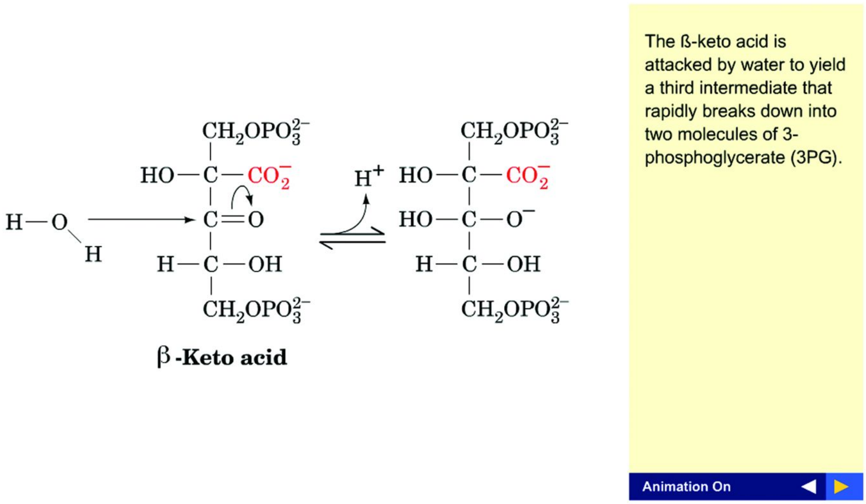

Figure 11. Rubisco drawings from Wiley for Voet and Voet (34). User does not interact with the structures. This is a flipchart presentation. This material is reproduced with permission from reference (34). Copyright 2012 Wiley & Sons, Inc.

The Wiley product does not provide new information for the student. The value of this supplement is that students have another way to read about the biochemistry. The "animations" are available at no cost online at www.wiley.com/college/fob/anim/index.html.

5. BrooksCole Animations

Perhaps the most useful publishing company animations for biochemistry come from the BrooksCole website. It is not immediately clear who deserves credit for the product. The animations are produced as drawings, so they are obviously not accurate. The eight topics that are presented are likely to be relevant in a typical biochemistry course. Motion is shown as moieties are transferred from one position on a protein structure to another. The chemistry that occurs is presented rather quickly, and many intermediates are left out of the animations; but by watching the animations, the overall process is clarified.

Program Attributes

The BrooksCole product is easy to use. It does not appear to be linked to a particular text. Representing a complete enzyme cycle is a significant challenge, and this teaching tool accomplishes that task for four systems (citric acid, pyruvate dehydrogenase, protein synthesis, and redox pathways of fatty acid and phosphorylation). Access to the animations is free.

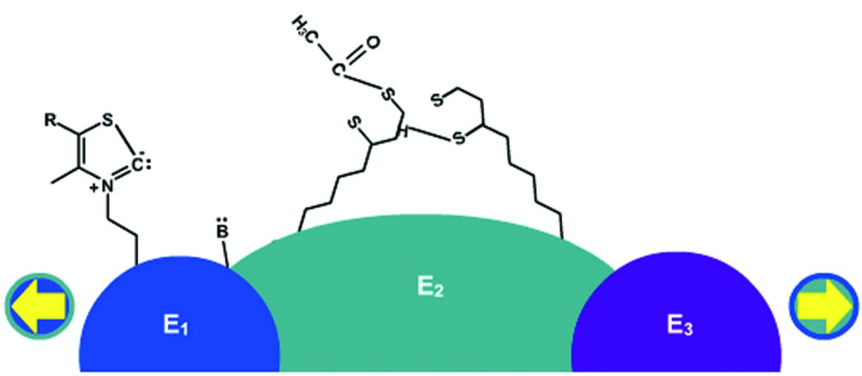

Figure 12. A screen capture of the BrooksCole animated transfer of hydrogen from one sulfur to another in the pyruvate dehydrogenase animation (35). From www.brookscole.com/chemistry_d/templates/student_resources/shared_resources/animations/pdc/pdc.html. ©. a part of Cengage Learning, Inc. Reproduced by permission. www.cengage.com/permissions

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Improvements

Perhaps this product shouldn't be included in the comparison provided in this paper. There is very little that is truly animated and it is not shown with any intent to be accurate (Fig. 12). Reactions are drawn without showing the reactive intermediates or the mechanisms. Access to this program is available at www.brookscole.com/chemistry_d/templates/student_resources/shared_resources/animations/#.

Conclusion

This chapter has presented an evaluation of five organic chemistry and five biochemistry visualization tools. The intent has been to inform the reader about the available tools, as well as to present the merits and shortcomings for each of these tools. Although the real value of the software in each case is difficult to ascertain, the final analysis must be: Does this teaching tool help the student learn the material? In each case I think the answer is yes.

Organic chemistry animations:

- Organic Reaction Mechanisms, by Montana and Buell
- Organic Reaction Animations, by Fleming, Hart, and Savage
- ChemTube3D, by Greeves and Berry
- Spartan, by Wavefunction
- Mol4D, by Borkent

Biochemistry animations:

- Bio-Organic Reaction Animations, by Fleming and Savage
- Individual products, by Dunham and Kyrk
- BME3D, by Martz and Herraez
- Biochemistry textbook animations, by Wiley
- Biochemistry animations, by Brooks/Cole

Acknowledgments

I appreciate the assistance of Ashley Augustyniak, the reference librarian at the Chemical Heritage Foundation.

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2. Authors of *Biochemistry* in alphabetical order: Berg, Tymoczko, & Stryer; Campbell & Farrell; Garrett & Grisham; Horton, Rawn, & Moran; Lehninger, Nelson, & Cox; Mathews, van Holde, & Ahern; Voet, Voet, & Pratt.
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10. ochem.jsd.claremont.edu. The user clicks on a reaction; and the process is shown one step at a time, each step showing arrow pushing after the user clicks on the window.
11. 3-D images help with depth perception issues.
12. Contact Sheri Strickland at sheri.strickland@converse.edu.
13. Ty Redd is a Professor of Chemistry at Southern Utah University. He is an outstanding instructor and he is always current with the latest teaching tools.
14. The student animators: Josh Harr, Paul Adams, Darrell Hurt, Brent Fielding, Alan Cheney, Jaron Hale, Matt Traynor, Doug Stewart, Stephen Cox, and Nathan Cahoon.
15. Presented at the National ACS Fall Meeting, Las Vegas, Sept. 1997, CHED #73.
16. The process has been described in more detail in Fleming, S. A.; Savage, P. B.; Hart, G. Molecular Orbital Animations for Organic Chemistry. *J. Chem. Educ.* **2000**, *77*, 790–793.
17. A product of Wavefuction, Inc. Although the AM1 level was used for most of the calculations, some reactions required ab initio level calculations.
18. Students benefit from 3D images of organic reactions. See Kitchen, L. K.Research Study of an Interactive CD-ROM for Teaching and Learning Organic Reactions. Brigham Young University Honors Thesis, 2000.
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20. Good news for the ORA fans. W. W. Norton has a beta version of an online multi-platform compatible product. The goal is to make it compatible with portable electronic devices.
21. Alex Lawrenson, Richard Windsor, Kirsty Barnes, Sze-Kie Ho, Louise Phillips, Lyndsey Vernon, Hannah Godfrey, Daniel Meadows, Smaher Butt, Suzanna Hussain, Ajay Antichen, Iain Aldous, Adam Byrne, Frances Potjewyd, Emma Schore, and Aled Roberts.

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27. For more information about this software, see: www.cacheresearch.com/home.html.
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34. This particular screenshot comes from www.wiley.com/college/fob/quiz/quiz18/18-22.html. The flip chart type presentation is associated with the Voet, D.; Voet, J. G.; Pratt, C. W. *Fundamentals of Biochemistry*; J. Wiley & Sons: 2012. The animations were created by S. B. Vik and executed by SuperNova Productions, New York.
35. This particular screenshot comes from www.brookscole.com/chemistry_d/templates/student_resources/shared_resources/animations/pdc/pdc.html.

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Chapter 17

Using Visualizations of the Science Behind Climate Change To Change the Climate of Science Teaching

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Simulations and other visualizations have been created to communicate the science of climate change to students in undergraduate chemistry and physics courses. Concurrent goals are to use climate science as a rich context for the teaching of fundamental science concepts, while also increasing climate literacy. An overview of our best practices for the use of visualizations is presented, followed by seven examples of simulations related to climate science developed at the King's Centre for Visualization in Science to introduce a diverse set of topics into undergraduate science classrooms.

Introduction

Climate Science as a Rich Context for Science Teaching?

The US Interagency *Climate Literacy* initiative (*1*) suggests that over the next several decades encompassing the professional careers of the students who are currently entering university classrooms, climate change is expected to have a substantially increasing impact on human and natural systems - affecting human health, biodiversity, economic stability, national security, and accessibility to food, water, raw materials, and energy. To prepare graduates to adapt to these new conditions (and benefit from new economic opportunities they create) will require both the ability to understand climate science and the implications of climate change, as well as the capacity to integrate and use that knowledge effectively.

Yet there is a pervasive and global disconnect between actual climate science knowledge and perceived knowledge (*2*). Research in the fall of 2012 on public attitudes and misconceptions about climate change (*3*) shows that 70% of American adults believe that climate change is happening, and for the first time since 2008, just over half (54%) attribute this mostly to human activity. Awareness and concern is higher in other regions of the world, including Latin America, India, and Europe (*4*). But without a solid public understanding of the causes of anthropogenic climate change and potential solutions, individuals are left with "overwhelming, frightening images of potentially disastrous impacts, no clear sense of how to avert this potentially dark future, and therefore no way to direct urgency toward remedial action" (*5*).

A review of five decades of science education relating to climate in general and climate change in particular demonstrates that basic climate science has not been well addressed at either the K-12 or post secondary levels in national and state education standards or science education curricula. Key misconceptions and misinformation about basic climate science; the role of human activities and reliance on fossil fuels on the climate system; and the consensus among the climate research community about the issues, are commonly held by students, teachers, politicians, and members of the public (*6*). Global studies corroborate these findings (*4*).

Analysts have concluded that climate change science, with its complex links to both natural processes and human activity, has fallen into a systemic hole in the science education system (*6*). Relegated to a subtopic of weather in many K-12 classrooms, climate change science has traditionally not been explicitly addressed in a substantial way in national science standards. Despite the commitment of over 600 US University and college presidents (*7*), the fractionation of knowledge at the undergraduate level poses additional challenges to moving the bar toward climate science literacy for students who come from high school with poor understanding of climate science fundamentals. For a variety of reasons, undergraduate biology, chemistry, and physics curricula have been reticent to address this defining educational and interdisciplinary global challenge.

As articulated in an NSF workshop on Chemistry for a Sustainable Future (*8*), modern chemistry is defined by its interdisciplinary boundaries, some of the most important of which (energy, green chemistry, and the environment) play pivotal roles in the quest for sustainability. Yet, with some exceptions (*9*, *10*), the evolution of resources to support context-rich learning about complex systems such as our planet's changing climate has lagged far behind the new frontiers in research.

Climate Science Is Complex Science

Apart from the need to achieve climate literacy, understanding complex systems is fundamental to developing an authentic understanding of science, and understanding is needed to guide responsible action. Climate change represents a classic complex system. "The spatial scale is global; the time scale dwarfs normal human concerns; and the dynamics of the climate are exquisitely complex and imperfectly understood" (*11*). The complexity of systems such as our climate makes them difficult to understand because they are composed of multiple interrelated levels that interact in dynamic ways (*12*). Additional pedagogical challenges are introduced by the requirement for learning concepts from different disciplines. Learning science through complex systems poses major pedagogical challenges, particularly to disciplinarily oriented undergraduate science education that is delivered primarily by conventional lecture-based pedagogies. This challenge calls for new tools and new resources to help learners cross disciplinary boundaries, and new inquiry-based pedagogies to facilitate learner engagement with complexity (*13*).

A Role for Visualization in Understanding Complexity

Structure-Behavior-Function theory (SBF) research on differences in expert-novice understanding of complex systems (*12*) suggests that the largest differences in understanding between expert and novice groups is in understanding causal behaviors and functions. Making connections among different levels of a complex system increases working memory load, and requires mental simulation to construct complete mental models (*14*, *15*).

Many of the concepts underlying the science of climate change require learner conceptual understanding resulting from the use of informed imagination to construct robust mental models. Think of the challenge for a first year university student trying to imagine correctly how 'greenhouse gases' function at the molecular-level as an anthropogenic driver for earth's changing radiation balance. A robust mental model requires the synthesis of fundamental knowledge about the interaction of electromagnetic radiation with molecules, leading to the ability to picture interaction of trace amounts of colorless carbon dioxide gas with invisible infrared radiation, and subsequent interaction of vibrationally excited carbon dioxide with IR-inactive atmospheric nitrogen and oxygen gases causing tropospheric warming. Sterman (*16*) suggests that barriers to comprehending the dynamics of complex systems such as climate include the difficulty we have recognizing and understanding feedback processes, underestimations of time delays, lack of understanding of basic principles of accumulation and how nonlinearities can create regime shifts.

Achieving climate literacy in the framework of complexity brings an opportunity for science education to embrace pedagogies shown by research to facilitate student engagement with and understanding of science concepts. Our overall approach is situated in active learning approaches, and our development of pedagogical tools is based on the demonstrated effectiveness of misconception-informed (*17*) interactive visualizations (*18*), case-based approaches (*19*), and guided inquiry strategies (*20*) in supporting student learning. These pedagogical approaches are becoming more widely accepted and used in undergraduate science courses. Yet the limited availability of context- and content-rich resources that are linked to curricular learning outcomes in introductory post-secondary science courses is a significant barrier to more widespread adoption of new pedagogical approaches.

The work described in this chapter seeks to fill that gap, by giving students an evidentially rooted understanding of some basic concepts of climate change while at the same time completing existing curricular goals in chemistry, physics, and other science courses. Some of the exemplars given could be applied to the teaching of science at the high school level while others may be more appropriate to college/university level presentations. In the context of the other work presented in this book, these exemplars are also intended to catalyze discussion within the scientific visualization community of best practices in the development of visualizations to facilitate the teaching and learning of complex science.

A Crucial Role for Visualizations

Visualization tools play a crucial role in our strategies to use climate science as a rich context for the teaching of fundamental concepts in science. The digital learning objects (DLOs) developed at the King's Centre for Visualization of Science described in this chapter, consist of one or more robust applets (small web transmissible computer simulation or visualization) that are supported by ancillary digital materials (learning outcomes, lessons, narratives, case studies, implementation strategies, etc). While each DLO integrates and packages these different pieces, the core applets provide the necessary interactivity by learners to enable the kinds of pedagogical practice that literature suggests are effective in supporting student learning (*21*). Both components are crucial for successful implementation in the classroom: the creation of robust interactive applets, and the careful integration of these into a suite of supporting materials that enable a user to tailor the implementation of any DLO to a variety of teaching and learning styles. Evidence suggests that the use of visualizations can make perceptible and cognitively tractable information that might otherwise remain opaque (*21–24*), and that visualizations can clearly enhance learning (*21*).

The DLOs include resources to facilitate their use by teachers and learners with a variety of teaching and learning styles, including guided inquiry- and case-based approaches. Evidence suggests that learners benefit from student-centered approaches in which they are encouraged to "practice and implement the processes and thinking skills associated with the work of professional scientists" (*25*, *26*). Case based approaches, used widely in medicine and law (*27*), may lend themselves particularly well to the introduction of complex science, such as the science of climate change.

In developing and implementing these DLOs, we have been guided by a set of best practices in the design of visualizations, which have been informed both by research on effective use of visualizations (*28*, *29*) and our own experience over more than 15 years with piloting numerous DLOs with secondary and post-secondary educators in workshop settings, and receiving subsequent feedback from those educators after they use the DLOs with their students (*30*). Those best practices include:

- Web-delivered DLOs should be designed to fully exploit the benefits of electronic delivery. These benefits include interactivity, and visually rich ways of engaging users with both data and models to explain data through simple yet intuitive graphical user interfaces.

- Rather than telling users what to think about complex systems, they can be invited to interrogate data sets and guided through a series of questions that allow them to understand what we know, as well as the limits of our knowledge.
- Materials can be designed to frequently provide self-checks of user understanding, and to discourage rapid "clicking" through a rich resource.
- Learning outcomes that address core scientific concepts as well as climate literacy goals are articulated prior to the development of materials on any topic.
- Relevant literature on student conceptual understanding and common misconceptions related to both core scientific concepts and climate literacy is surveyed, and DLOs are developed with specific goals to address prior understanding and misconceptions.

New Visualizations of the Science Behind Climate Change

One of the known barriers to addressing climate change in the classroom is the lack of easily accessible and usable curricular materials. We describe two sets of resources, Visualizing and Understanding the Science of Climate Change (www.explainingclimatechange.com) and Visualizing the Chemistry of Climate Change (www.Vc3chem.com), that we have developed with partners to make the complex science of climate change more tractable in the classroom and to provide interesting and motivating contexts for teaching basic science concepts. Explainingclimatechange.com targets a global audience of 16-19 year olds and their teachers. Vc3chem.com is designed for first year students in North American general chemistry courses and their instructors.

Visualizing and Understanding the Science of Climate Change (www.explainingclimatechange.com)

The King's Centre for Visualization in Science (KCVS), guiding an International Union of Pure & Applied Chemistry project, in partnership with The Royal Society of Chemistry, The American Chemical Society, and UNESCO has developed an interactive, on-line resource – *Visualizing and Understanding the Science of Climate Change*. This teacher/student-friendly set of resources, created as an International Year of Chemistry-2011 legacy, targets students between the ages of 16 and 19 years and comprises nine lessons. Figure 1 is a splash screen from this resource. Each lesson contains interactive simulations, video and assessment items. These could be used as either stand-alone teaching packages or as resources for adaptation to the classroom. Each lesson includes identification of key concepts as well as "test your knowledge" items. An extensive on-line glossary also assists students and teachers in navigating the at times jargon-laden world of climate change. All of the lessons operate within a custom-made content delivery system. This set of lessons is organized by climate literacy topics, but uses basic concepts in chemistry (and physics) curriculum at the Grade 12 or first year university level to increase understanding of the climate topics.

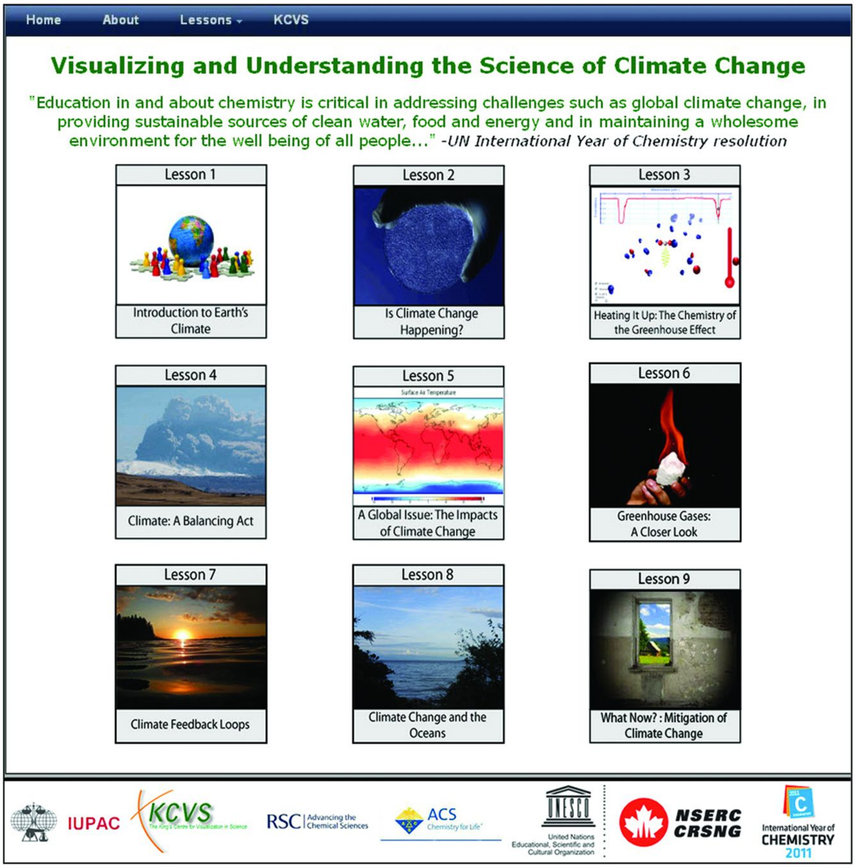

Figure 1. Splash screen from the ExplainingClimateChange.com site which is freely available to all teachers. (see color insert)

Visualizing the Chemistry of Climate Change (VC3Chem) (www.Vc3chem.com)

In 2011, with the support of NSF CCLI # 1022992, a partnership involving the King's Centre for Visualization, Purdue University and the American Chemical Society was assembled to develop and disseminate a series of interactive, web-based DLOs to help first year undergraduate chemistry students visualize and understand the chemistry underlying global climate change. The project carried out an extensive survey of core concepts in climate change science and topics taught in general chemistry in most US colleges and universities. Data was obtained from course syllabi from a number of leading institutions, and topics presented in eight leading textbooks were analyzed. A concept map

In Pedagogic Roles of Animations and Simulations in Chemistry Courses; Suits, J., et al.; ACS Symposium Series; American Chemical Society: Washington, DC, 2013.

was developed to link seven key climate change topics identified in *Climate Literacy – the essential principles of climate science* (*1*) with core topics in general chemistry. This inventory has helped shape *Visualizing the Chemistry of Climate Change* (VC3Chem) which, when completed, will provide instructors and students with an interactive database that links digital learning resources addressing key chemistry topics with corresponding climate change ideas (and vice versa). This will facilitate the creation of rich learning contexts that will encourage instructors to use climate change ideas as part of the daily "fabric" of teaching.

VC3Chem will also have an embedded research capacity that will allow us to monitor and assess student misconceptions relating to climate change. This will enable us to augment existing inventories of climate change misconceptions and aid in the design of more effective visualizations and simulations. The interactive DLOs have been introduced to educators at workshops held at three international chemistry education conferences in 2012: The joint International Conference on Chemistry Education/European Conference on Research in Chemistry Education in Rome, the Biennial Conference on Chemistry Education in Pennsylvania, and the Latin American Chemistry Congress in Cancun. Following these workshops, the resources are now being piloted in North American university and college classrooms, using appropriate tools to measure whether students using the materials demonstrate gains in understanding of both core chemistry and climate science concepts.

In developing these two sets of resources, we have been informed by other rich visualizations and in-depth discussions of many diverse aspects of global climate change. Three examples are: The NASA Earth Observatory (http://earthobservatory.nasa.gov/), The National Oceans and Atmospheric Administration Climate Service (http://www.climate.gov/#climateWatch) and Real Climate (http://www.realclimate.org/).

In the rest of this chapter, we show how resources from ExplainingClimateChange.com, VC3Chem.com, and our own teaching can be used to develop rich context exemplars to introduce climate change topics into traditional physics and chemistry undergraduate curriculum. The intent here is "symmetric" – climate change ideas will help bolster the acquisition of key concepts in physics and chemistry, while at the same time students will acquire understanding of the evidence for and science behind climate change. And because the visualizations are interactive, they provide resources to support changing the climate of classrooms toward increasing student engagement and ownership of material.

Historical Trends – The Mathematics of Change

Understanding trends and interpreting graphical data is a critical skill in the sciences. While concepts such as slope and rate of change are staples of mathematics curricula, these same concepts and skills require reinforcing in the science classroom. As an example consider historical records of atmospheric CO_2 concentration and temperature derived from proxy measures applied to ice cores. Figure 2 shows a temperature plot derived from Antarctic ice core data which spans 800 ka of Earth's history. This is part of the visualization *Climate Trends*. Prominent in the graph are the seemingly rapid temperature changes from glacial to inter-glacial periods. The highlighted region shows a period of rapid warming. An interactive slope tool enables a student to measure the rate of change and conclude that the average rate of change implied is roughly 0.001 $K \cdot a^{-1}$. If the same tool is then used to measure the average rate of change over the past 100 years the student finds, remarkably, that the current rate of change in temperature is more than an order of magnitude greater than this. This not only helps to underscore the importance of interpreting what a slope means but also helps point out that in understanding evidence for anthropogenic climate change (and why what we observe today is not a repeat of similar events in past epochs); the ***rate of change*** is very significant. This point is illustrated in Figure 3a and 3b in which data from the last 100 years is presented.

In these panels the issue that easily confuses students is that of scale. A cursory glance at the temperature-time graph in Figure 3a would suggest that there has been only a slight warming over the past century and certainly less dramatic than the trend shown in Figure 2.

When the data is re-scaled, however, and slope determined a very different story emerges. Now the rate of change over the past 100 years is an order of magnitude greater than the data investigated from a much earlier epoch.

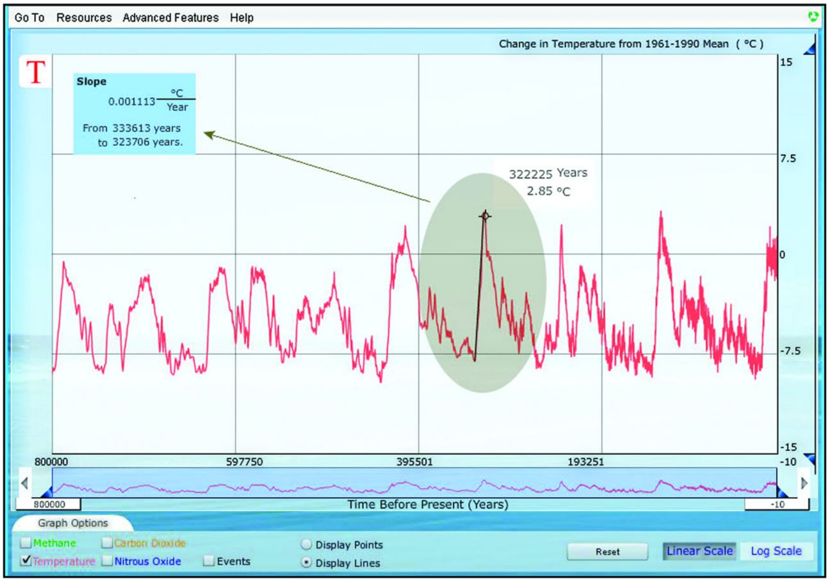

Figure 2. Panel from the applet Climate Trends showing historical temperature records obtained from ice core data. (http://www.explainingclimatechange.ca/Climate%20Change/swf/climatetrends/historyGraphs.swf)

(a)

(b)

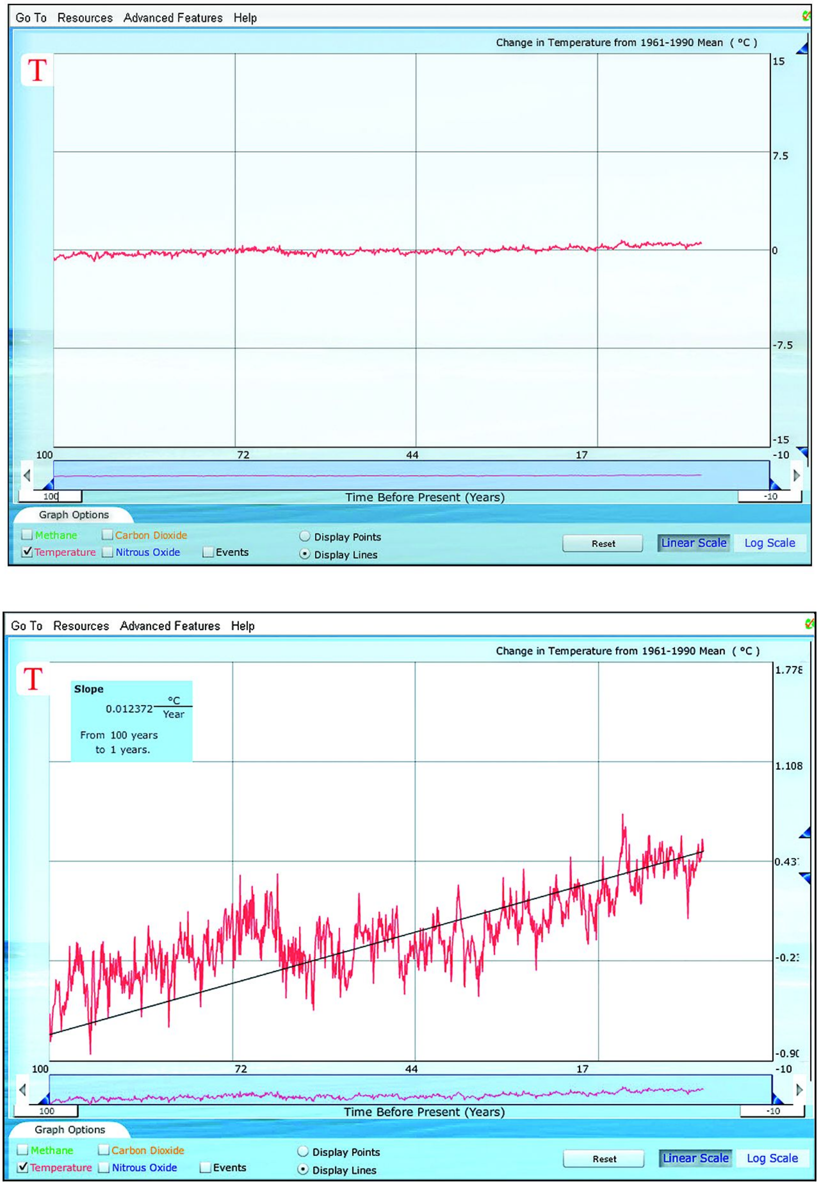

Figure 3. (a) Temperature – time data for the past 100 years without scaling of vertical axis. (b) The same data as part (a) but now scaled in the vertical axis.

As another example of how climate change ideas can help provide insight into interpreting graphical information consider the meaning of the term "intercept" as it is applied to a graph of polar ice cover. Figure 4 shows the GUI for the visualization *Polar Ice* which shows September polar sea extent. With this applet a student is able to examine data collected from the National Snow and Ice Data

Center (NSIDC) for the period 1979 – 2010 (most current available at time of writing). The applet permits the student to measure the polar ice area and to plot the data and export this data to a spreadsheet or numerical analysis program.

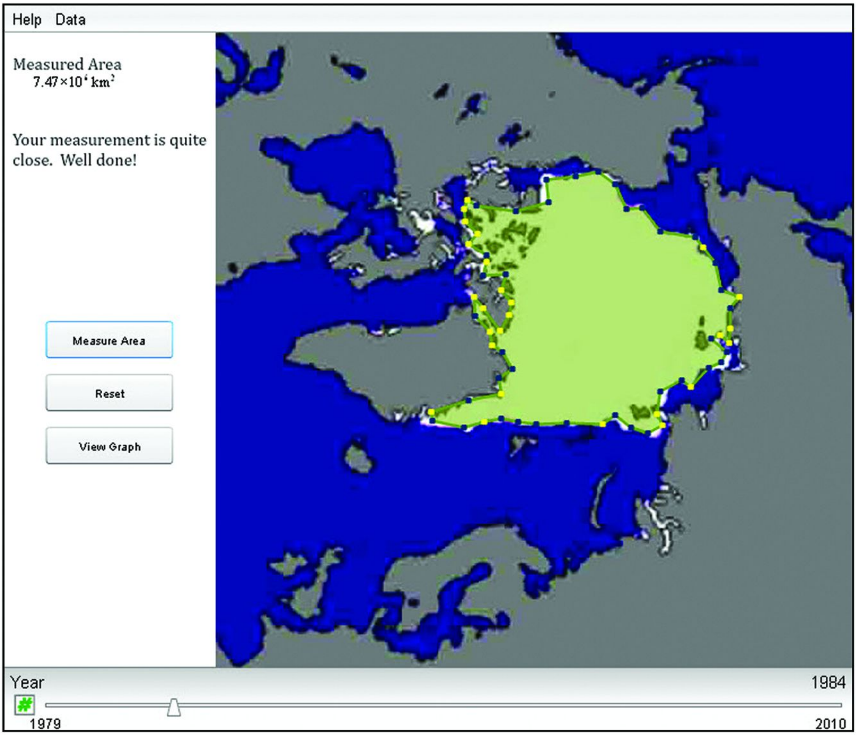

Figure 4. The graphical user interface for the applet Polar Sea Ice. The green region represents the measured region using a simple measuring tool. (http://www.explainingclimatechange.ca/Climate%20Change/swf/Polar%20Ice/Polar%20Ice.swf)

As an example the sea ice coverage data from this visualization was exported and graphed (Figure 5) in EXCEL. A subsequent trendline analysis for the extent of late summer sea ice yields the equation

$$A(t) = -0.0914t + 8.0744$$

where A(t) represents area of late summer sea ice as a function of time 't' from the year 1979. The x-intercept of this graph can be easily found to occur when t = 88.3 years after 1979. In other words – if this trend is maintained it is projected that by the year 2067 the arctic will be ice free by late summer. This discussion would help not only reinforce the message that the features of graphs (slopes and intercepts for example) have physical meaning but could also prompt a discussion on the potential risks of extrapolating or "future-casting" data.

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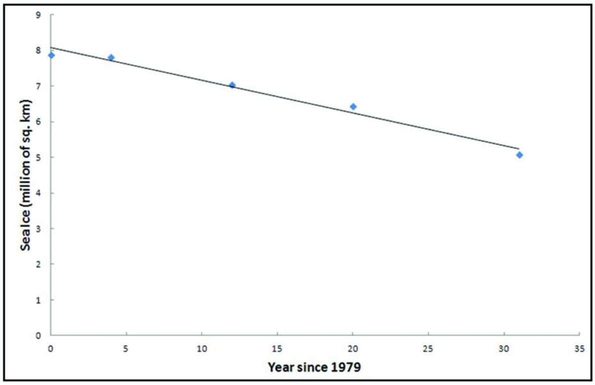

Figure 5. Trendline fit to data collected with applet Polar Sea Ice.

An important motif in most of the visualizations and simulations presented here is the importance of student engagement with data and ideas. By "playing" with data such as the temperature or sea ice records shown above students can develop more robust understanding of how to manipulate data and at the same time gain insight into some of the principal reasons for concern in understanding global warming.

The Physics and Chemistry of the Atmosphere

The Atmosphere

Students (and the general public) sometimes express incredulity when faced with the idea that we can actually have an impact on the atmosphere – it "seems so big". To help students visualize the fragile nature of the troposphere a simple activity is to consider the relative size of the earth to the thickness of the troposphere – the region in which most climate and weather effects occur. The thickness of the troposphere is approximately 10 km while Earth's radius is roughly 6000 km. How would you draw this? Draw a circle 25 cm in radius on a white board in a lecture hall. The troposphere can then only be $(1/600)^{th}$ of this or less than one-half a millimeter thick! The late Carl Sagan liked to use the apt analogy that the part of the atmosphere that matters most is roughly the thickness of the shellac layer on the surface of a school room globe. When visualized this way it becomes much more plausible that we could have an impact on the atmosphere.

In addition to scale of the atmosphere there is a great deal of subtle chemistry involved in the structure of the atmosphere. Figure 6 shows the graphical user interface of the visualization *Structure of the Atmosphere*. This interactive tool allows students to explore the four main regions of the atmosphere and also to begin to see how chemical substances and their interactions with electromagnetic radiation help to define these regions.

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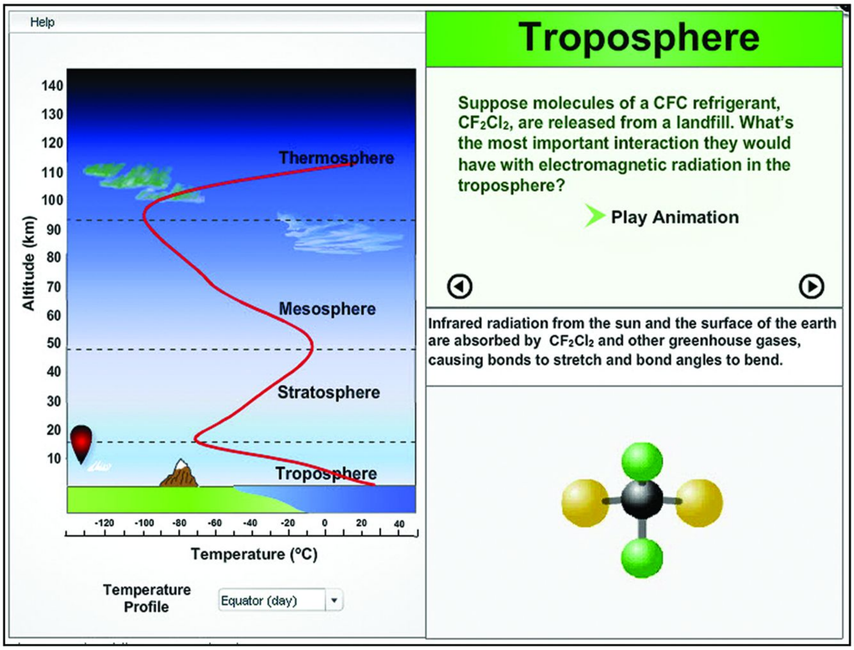

Figure 6. The graphical user interface for the visualization Structure of the Atmosphere (http://www.explainingclimatechange.ca/Climate%20Change/swf/atmosphere/atmosphere.swf)

The text shown on the right in Figure 6 is a discussion of the interaction of electromagnetic radiation with CFCs in the atmosphere. This discussion can enhance a student's understanding of why CFCs are harmful agents in the atmosphere, and how they interact very differently in the troposphere and stratosphere. This thread could be continued with the simulation *CFCs in the Atmosphere* shown in Figure 7. This interactive simulation allows students to explore the relation between wavelength of electromagnetic radiation and the mode of interaction with a CFC molecule.

Calculating the Mass of the Atmosphere

Physics and chemistry are at their best when, with simple tools and very basic information, a student can discover something "remarkable". One of the most basic ideas in understanding climatic changes in atmospheric temperature requires that we know the mass of the atmosphere. While this may seem to be a complex task it is in fact accessible to students at a high school – introductory college level and can be achieved by developing a straight forward mental visualization. Start with a very basic piece of knowledge – atmospheric pressure. Many students will already know that the atmospheric pressure, at sea level, is roughly 100 kPa. Since 1 Pa is 1N/m^2 we know that each square meter of Earth supports a column of air

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weighing 100 kN. Applying Newton's second law leads to the result that each square meter supports 10^4 kg of air. The rest is simple geometry! The surface area of a sphere is given by

$$SA = 4\pi R^2$$

with R = 6.4×10^6m this leads to a mass of

$$M = (10^4 kg / m^2) 4\pi (6.4 \times 10^6 m)^2 = 5.1 \times 10^{18} kg$$

If students haven't already challenged you on this you may want to ask them what assumptions have been made in this calculation. The most obvious is the assumed constancy of "g", the local acceleration of gravity. Since roughly 98% of Earth's atmosphere is contained in the bottom 30 km you could ask students to estimate how big an error you are making by using this assumption.

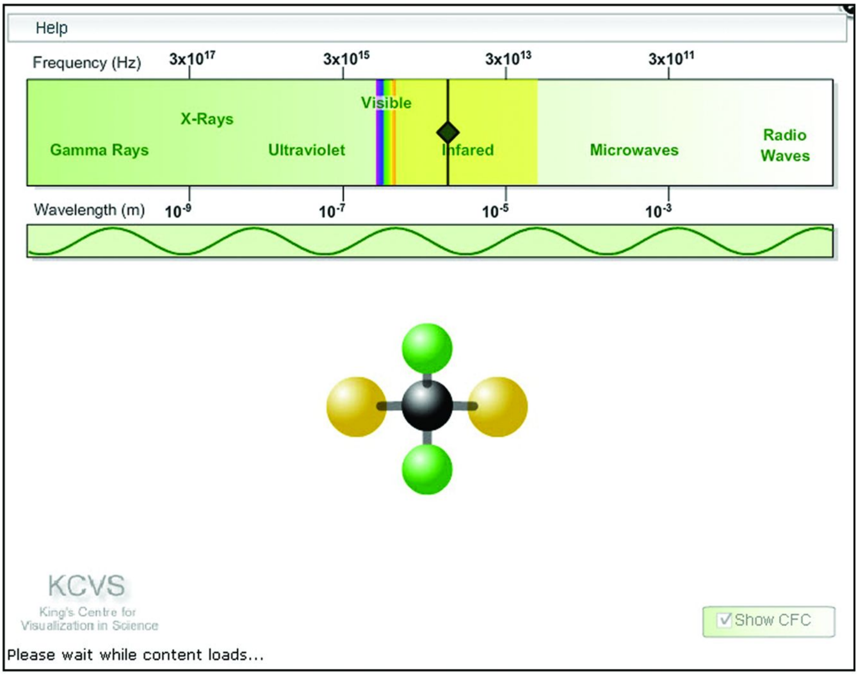

Figure 7. The simulation CFCs in the Atmosphere. (http://www.kcvs.ca/site/projects/common_files/CFC/cfc.swf)

Knowing the mass of the atmosphere, it is relatively easy to find the number of moles in the atmosphere. Since air is approximately 79% N_2 and 21% O_2, the "weighted average" atomic weight of air is 28.8 g/mol. The number of moles in the atmosphere is then

$$molar\ mass = \frac{5.1 \times 10^{21} g}{28.8\ g/mol} = 1.8 \times 10^{20} mol$$

Armed with this, a student can now begin to understand how to calculate the change in concentration of atmospheric CO_2 through the burning of fossil fuels.

Calculating Atmospheric CO_2 Concentrations

Most hydrocarbon-based fuels used today can be assigned the approximate chemical composition of octane (C_8H_{18}) or diesel fuel ($C_{12}H_{26}$ - $C_{16}H_{34}$). Let's assign a "typical" chemical formula of $C_{12}H_{26}$ to represent the starting material for burning a fossil fuel. By balancing the chemical reaction equation we can determine the amount of CO_2 produced in a combustion reaction for a particular amount of hydrocarbon:

$$2\,C_{12}H_{26}(g) + 37\,O_2(g) \rightarrow 24\,CO_2(g) + 26\,H_2O(g)$$

By comparing the molar masses of $C_{12}H_{26}$ and CO_2, students can readily understand the "leveraging" effect of fossil fuel combustion. Roughly 3.2 times as much CO_2 (by mass) is released when a certain amount of fossil fuel is burned. This can quickly lead to some revealing calculations. A typical barrel of oil has a mass of 135 kg and, when burned, releases 425 kg of CO_2. Another way to state this is that for every barrel of oil burned

$$\frac{425\ kg}{0.044\ kg/mol} = 9.7 \times 10^3 mol$$

9.7×10^3 mol of CO_2 are released. Since there are 1.8×10^{20} mol in the atmosphere, each barrel of oil, when burned, changes the atmospheric concentration of CO_2 by

$$\frac{9700\ mol}{1.8 \times 10^{20} mol} = 5.4 \times 10^{-17}$$

5.4×10^{-17}, which is equivalent to 5.4×10^{-11} parts per million (ppm).

Since 30 billion barrels of oil are burned annually, the expected increase in atmospheric CO_2 from oil burning should be on the order of 1.6 ppm. In reality only about 37% of the CO_2 produced comes from oil (40% comes from coal combustion and the rest comes from natural gas and the curing of concrete). The expected, annual change in CO_2 concentration is therefore about 4.8 ppm. How does this number relate to what we know about CO_2 concentration in Earth's atmosphere? Figure 8 shows the data for atmospheric concentration of CO_2 as measured from the Mauna Loa observing station between the years 1988 to 2009 plotted with an interactive tool created for the Visualizing and Understanding the

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Science of Climate Change site. The average rate of increase of CO_2 concentration over the past 20 years is 1.7 ppm· a^{-1}. This is the correct "ball-park" according to our calculations and also begs the question – if we calculated an increase of 4.8 ppm but see "only" an increase of 1.7 ppm· a^{-1}, where is the rest of the CO_2 going? This will be addressed in the section Carbon Dioxide and Changing Ocean Chemistry, later in this chapter.

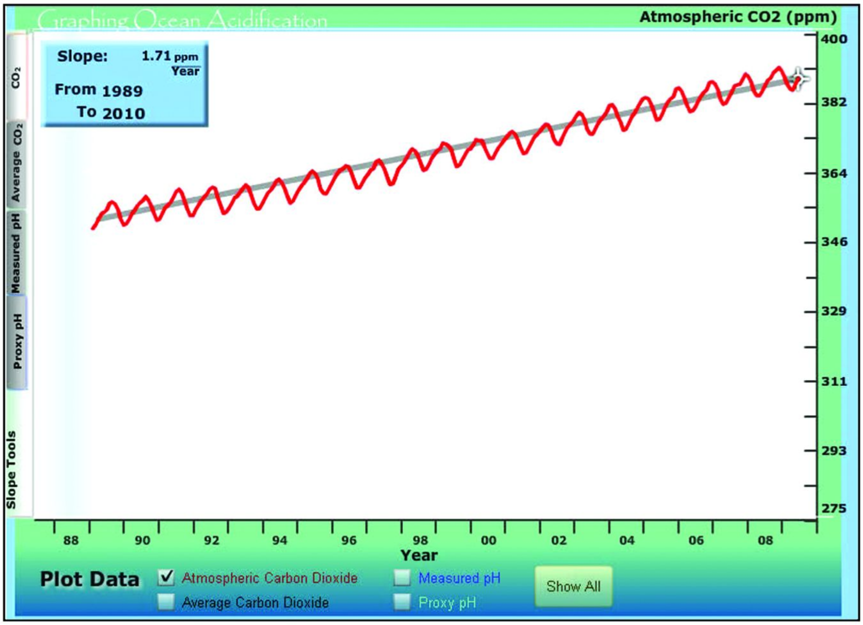

Figure 8. Variation of atmospheric CO_2 levels in ppm for the period 1988 – 2009. Data from applet Graphing Ocean Acidification (http://www.explainingclimatechange.ca/Climate%20Change/swf/pHKeelingCurveGrapher/pHKeelingCurveGrapher.swf)

Quantifying the Annual CO_2 Atmosphere-Biosphere Exchange

Inspecting the Keeling curve leads to an interesting insight into how much CO_2 is exchanged annually between the atmosphere and the biosphere (including ocean-atmosphere). Figure 9 shows a variation for the period late winter 2011 to late summer 2011. CO_2 levels drop from 394.2 ppm to 389.0 ppm for a total change of 5.2 ppm. Since the molar mass of the atmosphere is 1.8×10^{20} mol, the annual exchange of CO_2 amounts to 9.0×10^{14} mol or 41.2 GT. The insight gained is that this number is of the same magnitude as the current **additional** anthropogenic CO_2. While the ecosystem naturally accommodates a massive transfer of CO_2 annually, it cannot accommodate the additional anthropogenic burden and hence CO_2 levels must rise.

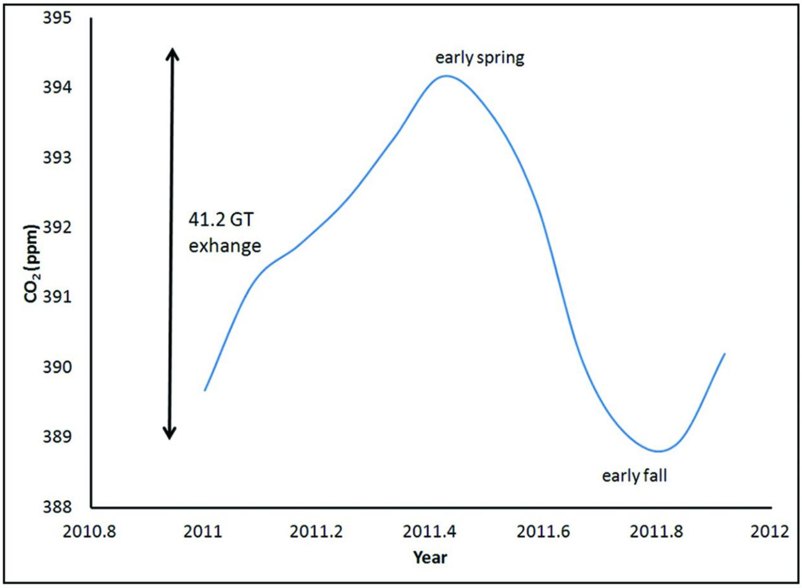

Figure 9. Variation of CO_2 levels during 2011 illustrating a net exchange of 41.2 GT of CO_2 during the year.

It should be noted that in these calculations Mauna Loa data was used and the results will be slightly different (lower) if globally averaged CO_2 concentrations are used.

Earth's Radiation Balance and the Greenhouse Effect

One of the first suggestions that gases in Earth's atmosphere may contribute to warming the planet came from Fourier in the 1820s. In 1896 Svante Arrhenius published the first paper actually identifying CO_2 as a greenhouse gas and calculated the heating effect that CO_2 has on warming the planet. In the next section we will address the mechanism by which greenhouse gases warm the atmosphere. In this section we look at the idea of radiation balance and present a simulation intended to provide students with a phenomenological understanding of greenhouse gas heating.

The simulation makes a very simple starting assumption – the globally averaged radiant energy from the sun is in equilibrium with thermal energy radiated back into space by Earth. This can be expressed via

$$E_{sun} = S_o(1-\alpha)\pi R_E^2$$

where S_o is the solar constant (1361 W·m^{-2}), α the albedo of earth (0.33) and R_E the earth radius. Since the earth is assumed to be in radiative equilibrium it follows, via the Stefan-Boltzmann Law that

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$$E_{earth} = 4\pi R_E^2 \sigma \varepsilon T_{eff}^4$$

where σ is the Boltzmann constant (5.67 × 10^{-8} $Wm^{-2}K^{-4}$), ε is the average emissivity of earth (set as 1 here) and T_{eff} is the average global temperature. Setting E_{sun} = E_{earth} yields the following:

$$T_{eff} = \sqrt[4]{\frac{S_o(1-\alpha)}{4\sigma\varepsilon}}$$

from which one gets an estimated global mean temperature of 252 K. When this is compared to the actual mean surface temperature of 288 K the greenhouse heating of 36 K is apparent. The simulation applet *Planetary Climate* invites students to experiment with the effect that greenhouse gas concentration and albedo will have on planetary temperature. In this simulation the greenhouse contribution is a dimensionless factor that does not have a direct relation to actual concentrations in ppm. Figure 10 shows the graphical user interface for this applet.

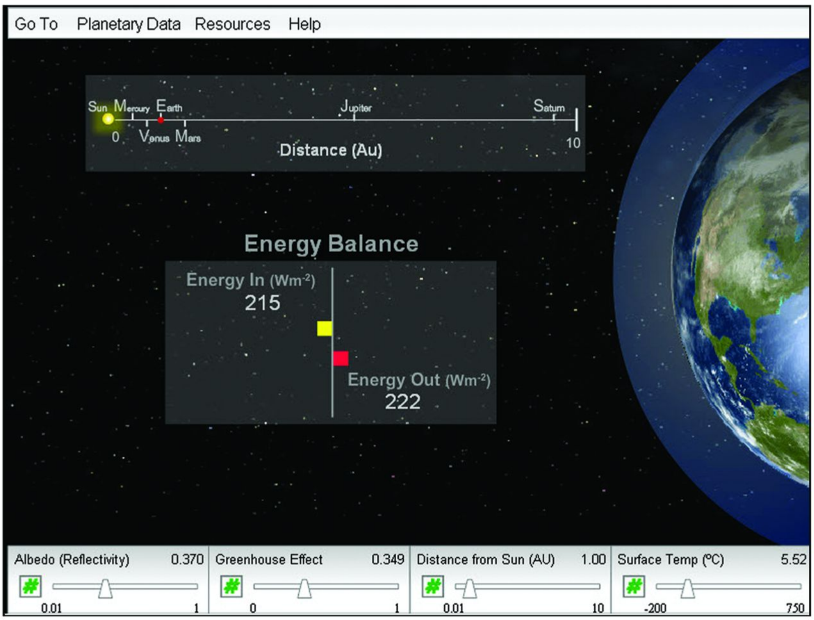

Figure 10. Interface for the applet Planetary Climate. (http://www.explainingclimatechange.ca/Climate%20Change/swf/radiationbalance/PlanetaryRB.swf)

Greenhouse Gases and Spectral Windows

How Greenhouse Gases Heat the Atmosphere

How does a gas such as CO_2 contribute to atmospheric warming? A commonly held view – and one often seen in visualizations – is that greenhouse

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gases scatter infrared radiation back toward the earth. While this can occur in the upper atmosphere it plays a negligible role in the troposphere. The actual mechanism behind greenhouse gas warming is in fact quite different and has to do with both the quantum nature of molecular absorption of electromagnetic radiation as well as the collisions that occur between molecules. A CO_2 molecule is able to absorb IR-radiation in selective wavelength bands. The molecule is able to undergo both stretching and bending mode vibrations when it absorbs infrared radiation that Earth radiates back into space. Most of this absorption occurs in the troposphere where the rate of molecular collisions is also very high. A relatively easy calculation shows that at 300 K and 1 atmosphere of pressure the mean time between collisions of air molecules is about 4.5×10^{-10} s. On the other hand, the transition lifetime for the CO_2 bending mode (between 600 – 800 cm^{-1}) is on the order of 0.5 s. Before an excited CO_2 molecule can re-radiate absorbed infrared radiant energy (i.e. scatter) it will undergo a collision with either N_2 or O_2 and lose this energy. This effectively transforms infrared radiation into translation energy of the gas in the atmosphere, hence "heating" the atmosphere. Figure 11 shows the simulation applet Collisional *Heating in the Atmosphere* available on the **Visualizing and Understanding the Science of Climate Change** web site that allows students to see how molecular vibration is wavelength dependent and how collisional de-excitation is able to transform IR- radiant energy into thermal energy.

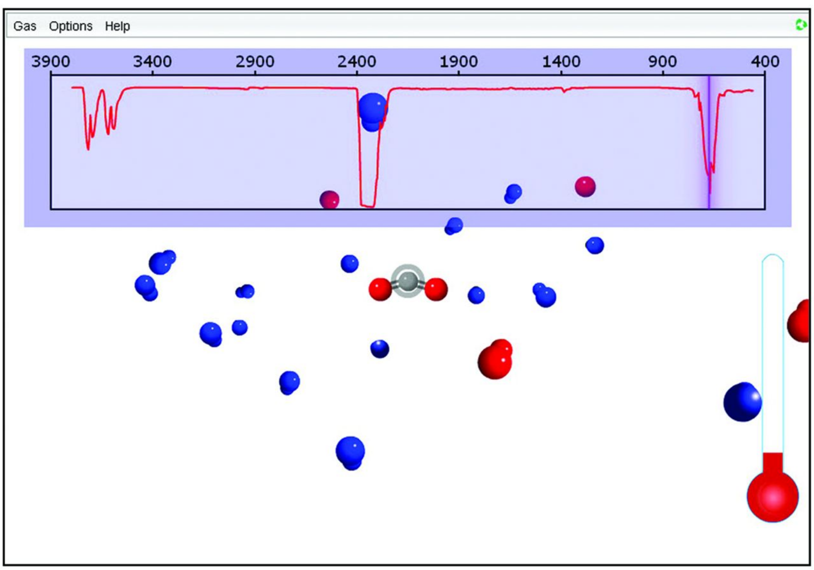

Figure 11. Interface from the simulation Collisional Heating in the Atmosphere shows a CO_2 molecule undergoing a bending mode vibration. (http://www.explainingclimatechange.ca/Climate%20Change/swf/videos/CollisionalHeating.swf)

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Spectral Windows and Greenhouse Gases

Earth receives energy from the sun in the spectral range that peaks around 550 nm (with the Sun radiating at 5800K) and emits back into space in the far infrared, peaking around 10 000 nm. Figure 12 shows a black body curve consistent with a mean global surface temperature of 288 K. Superimposed on this are absorption profiles for four prominent greenhouse gases: Water vapor (H_2O), carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) as well as a number of additional greenhouse gases (some with large contributions from human activity). The absorption bands for CO_2 are highlighted. Between the absorption lines are regions ("windows") through which infrared radiation can still pass and provide cooling to the planet. Note that many of these gases will absorb near the peak of Earth's blackbody emission and have the potential to cause significant warming even at low concentrations.

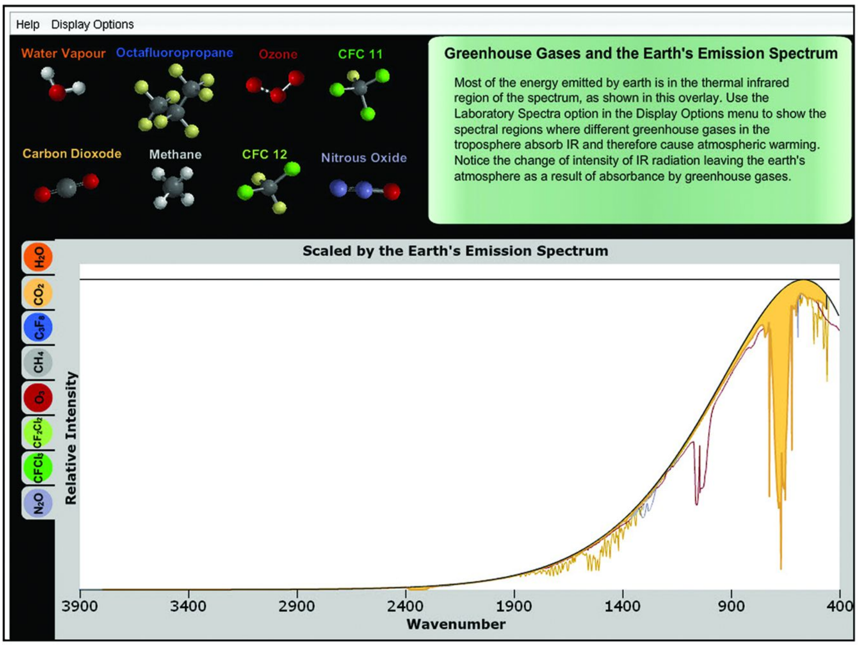

Figure 12. Interface from the applet Infrared Spectral Windows Absorption spectra of four important greenhouse gases shown in relation to the blackbody spectrum emitted by Earth's surface. (http://www.explainingclimatechange.ca/Climate%20Change/swf/irwindows/IRwindows2.swf)

These profiles have been scaled to fit the blackbody curve and illustrate their relative importance in blocking IR radiation in the atmosphere. The net effect is to close the spectral windows which will shift the radiative equilibrium of the planet to create a warmer atmosphere – i.e. global warming. Figure 12 was produced using the applet *Infrared Spectral Windows* available on the **Visualizing and Understanding the Science of Climate Change** web site.

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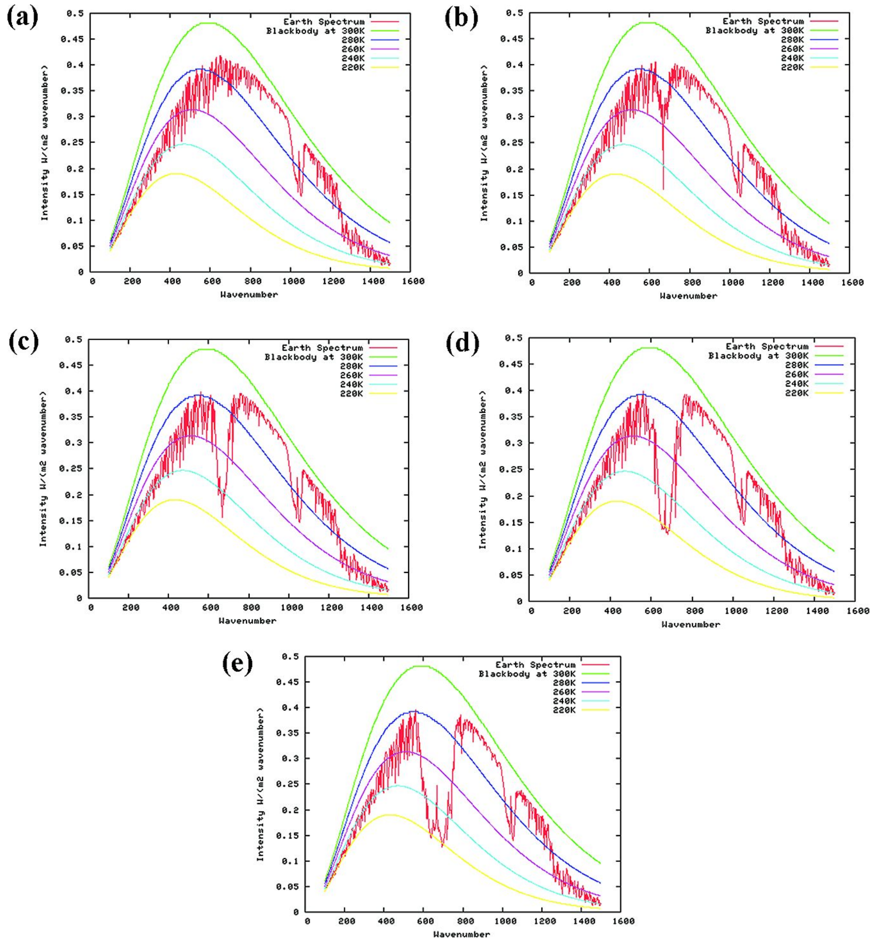

Figure 13. (a) CO_2 concentration 0 ppm. (b) CO_2 concentration 1 ppm. (c) CO_2 concentration 10 ppm. (d) CO_2 concentration 100 ppm. (e) CO_2 concentration 1000 ppm.

Absorption Band Saturation and a "Contrarian Canard"

A topic suitable for advanced chemistry and physics students is that of saturation effects in absorption bands created by CO_2 and other GHGs. The CO_2 band in the 600-800 cm^{-1} region provides a case-in-point. The term "saturation" is easily misconstrued and has often been used in contrarian arguments to suggest that CO_2 cannot absorb any more IR radiation since it is "saturated". Unfortunately this is not what the term saturation means when applied to a planetary or stellar atmosphere. A very effective visualization of this is provided by Archer (*31*). In this visualization a student has on-line access to the atmospheric absorption modelling program Modtran. Modtran (**Mod**erate Resolution atmospheric **tran**smission) is a sophisticated modeling package developed by Spectral Sciences Inc and the US Air Force that allows users to model the effects that atomic and molecular absorbers have on the transmission of radiation in Earth's atmosphere. Figures 13a-13e show a series of atmospheric transmission spectra created by Modtran for the 100 cm^{-1} – 1500 cm^{-1} region with CO_2 concentrations of 0 ppm, 1 ppm, 10 ppm, 100 ppm, and 1000 ppm respectively. These graphs show a marked difference in the band absorption for atmospheric concentrations between 1 ppm and 10 ppm. By the time one reaches a concentration of 10 ppm saturation effects are appearing. The absorption profile is flattening and broadening.

The term saturation refers to a change in the degree to which IR radiant energy is removed from the outgoing radiation from the earth below. At very low concentrations there is an approximately linear relationship between energy removed and concentration. By the time one reaches 10 ppm, however, the relation becomes logarithmic and this marks the transition to the saturation regime. Table I gives the atmospheric emission intensity in W m^{-2} at an altitude of 70 km and Figure 14 shows clearly that as one enters the saturation region and progresses from 10 ppm to 1000 ppm there is a monotonic decrease in energy transmitted.

Table I. CO_2 concentration and intensity of emission form Earth's atmosphere at an altitude of 70 km

CO_2 concentration (ppm)	*Radiated Intensity ($W{\cdot}m^{-2}$)*
0	318.396
1	313.843
10	305.522
100	294.061
1000	283.354

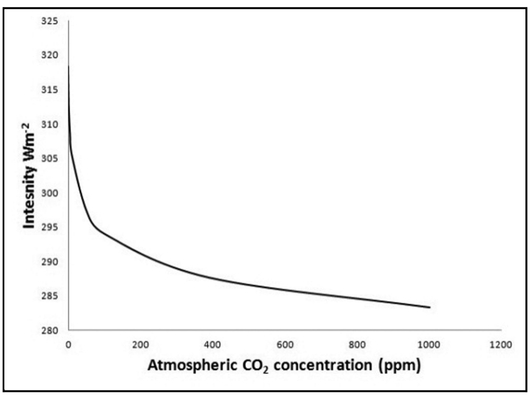

Figure 14. The relationship between increasing CO_2 concentration and reduction of transmitted radiant energy.

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Carbon Dioxide and Changing Ocean Chemistry

Ocean Acidification

One of the most disturbing discoveries in climate science of the past 20 years is the effect that increased absorption of human-generated CO_2 is having on the complex chemistry of Earth's ocean. Our previous calculations hinted that most of the CO_2 introduced into our atmosphere by fossil fuel burning was ending up elsewhere. Much of this "missing" CO_2 is being absorbed by the ocean. This is an excellent application of acid-base chemistry and can be simplistically characterized by the following reaction equations:

$$CO_2(g) + H_2O(\ell) \rightleftharpoons H_2CO_3(aq)$$
$$H_2CO_3(aq) \rightleftharpoons H^+(aq) + HCO_3^-(aq)$$
$$HCO_3^-(aq) \rightleftharpoons H^+(aq) + CO_3^{-2}(aq)$$

The ocean buffers atmospheric CO_2 through the interconversion of carbonic acid (H_2CO_3), bicarbonate, and carbonate ions (HCO_3^-, CO_3^{-2}). As CO_2 is absorbed into the ocean the buffering action of the ocean does some subtle things. Increased production of carbonic acid is accompanied by an increase in "acidity" (the number of hydronium ions (H^+)) and decrease in pH of the oceans. This in turn causes a shift in the equilibrium concentrations of bicarbonate and carbonate ions. Why does this matter? Marine organisms such as corals and mollusks secrete $CaCO_3$ in several different forms to form their skeletal material, and much of the base of the aquatic food chain is critically dependent on carbonate ion concentration. As the pH of the ocean drops, so too does the carbonate ion concentration, and the solid shells of certain marine organisms become soluble in water. Figure 15 shows an ocean acidification digital learning object from **Visualizing and Understanding the Science of Climate Change** that enables students and teachers to explore how changing ocean pH and speciation of carbon can be related to carbon usage as expressed in atmospheric CO_2 concentration.

To quantify this, consider the change in ocean pH since the Industrial Revolution. The pre-industrial revolution pH was 8.2 while today the ocean pH is 8.1. That doesn't sound like much of a change! But let's calculate how much the actual hydronium ion content ("acidity") of the ocean has changed.

By definition a pH of 8.2 is given by

$$pH = -\log_{10}[H^+]$$

So the hydronium ion concentration (pre-industrial) was

$$10^{-8.2} = 6.31 \times 10^{-9}\ mol\ L^{-1}$$

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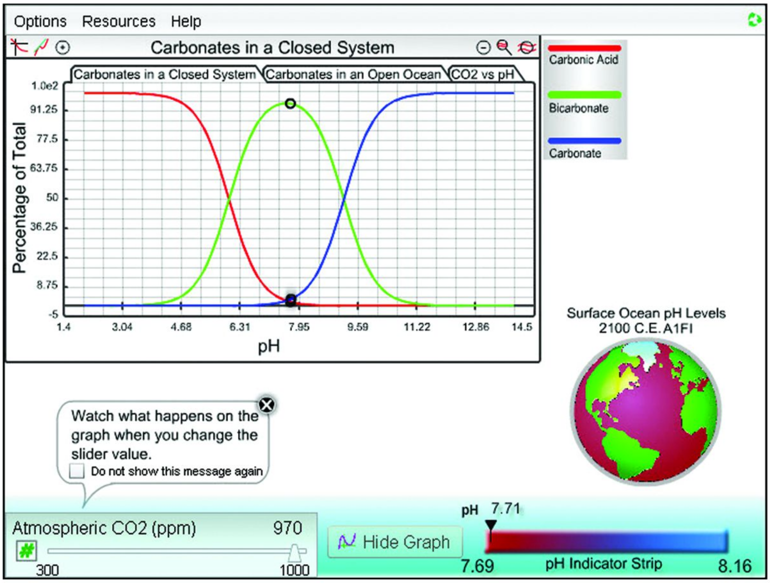

Figure 15. The applet Ocean Acidification which enables student's to explore the relationship between atmospheric CO_2 concentration and ocean chemistry. (http://www.explainingclimatechange.ca/Climate%20Change/swf/pHvsCO2Applet/pHCO2grapher.swf) (see color insert)

A pH of 8.1 corresponds to an $H^+(aq)$ concentration of 7.94×10^{-9} mol L^{-1}. This represents an increase of 25% in the acidity of the ocean. This is already (along with temperature and other effects) wreaking havoc on a wide variety of marine organisms including plankton and those found in coral reefs. Currently Earth's ocean is more acidic than any time in the past 20 million years! This will only worsen over the next century, unless addressed now.

Ice Cores and Isotopic Ratios (and Other Proxies)

Using Isotopic Ratios To Measure Temperature

Isotopes and isotopic ratios provide remarkable insights into Earth's climate and enable us to determine such things as the extent of ice sheets and air temperature in paleoclimate history. The isotopic ratio of oxygen atoms is one of the most useful proxies for determining temperatures of the distant past. Since ^{18}O is slightly heavier than ^{16}O, water that contains ^{18}O atoms will have slightly different physical properties than water containing "light oxygen". Water containing light oxygen evaporates more readily than water containing heavy oxygen; conversely water containing heavy oxygen condenses more readily. This means that as temperatures drop, so too does the atmospheric concentration of water containing heavy oxygen. Polar ice cores (either Greenland or Antarctic) provide us with "temperature museums". When the ice from a particular depth

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in an ice core is analyzed, a lower concentration of ^{18}O tells us that the ice was formed when temperatures were lower. By correlating ice core depth with time and ^{18}O concentration with temperature, climatologists are able to reconstruct Earth's climate history nearly 1 million years into the past. Deuterium isotope ratios are also commonly used to provide temperature proxies and Figure 16 illustrates the correlation between the change in deuterium (relative to a fixed standard) and temperature for ice sample taken from the Vostok ice core in Antarctica. The data spans 420 ka and shows a strong linear relation between change in isotope concentration and change in temperature. The Visualizing and Understanding the Science of Climate Change digital learning objects also include a very useful applet that allows students to investigate the Vostok and Dome C Antarctic data sets shows temperature, CO_2, N_2O and CH_4 ice-core data spanning nearly 1 million years of climate history.

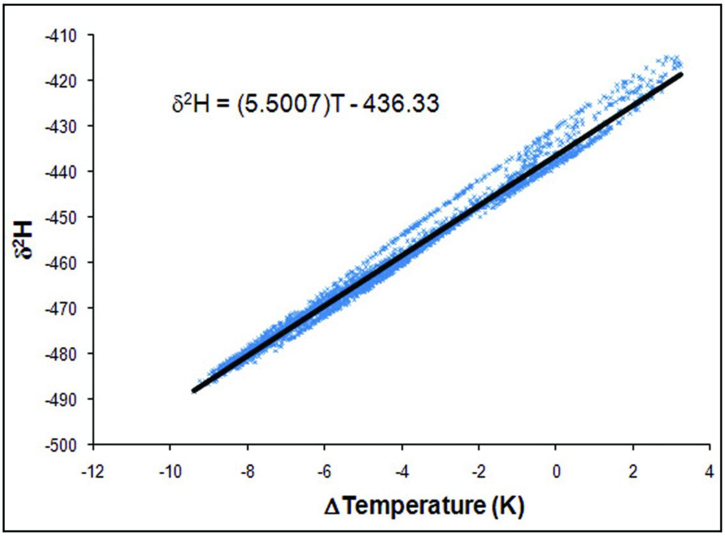

Figure 16. Linear relationship between change in deuterium abundance and change in temperature.

Mitigation Strategies - A Mosaic of Solutions

Decarbonization of Energy – An Exercise in Scaling Arguments

A fruitful discussion for an introductory chemistry or physics class could center on applications of the concept of energy. Aside from more formal treatments of the concept of energy there are many practical applications that help provide a sense of relevance for students. One example is to contrast carbon-based energy with alternate energy sources. Figure 17 shows the control panel of the applet Carbon Stabilization Wedges, which is modeled after the Princeton Carbon Stabilization Wedges developed by the Carbon Mitigation Initiative (*32*). The

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underlying idea of carbon stabilization "wedges" is to reduce annual carbon emissions by approximately 8 GT and to stabilize atmospheric CO_2 levels at their current (2012) value. One lesson from this is that there is no single solution or technology that can accomplish this – however, a mosaic of solutions using existing technologies can accomplish this goal. A user can make changes in a four major categories: Efficiency, Decarbonization of Power, Decarbonization of Fuel and Forest and Agricultural Soils Management. The applet not only calculates the carbon saving but also whether the proposed change is realistic. Behind all of these calculations are relatively simple scaling arguments.

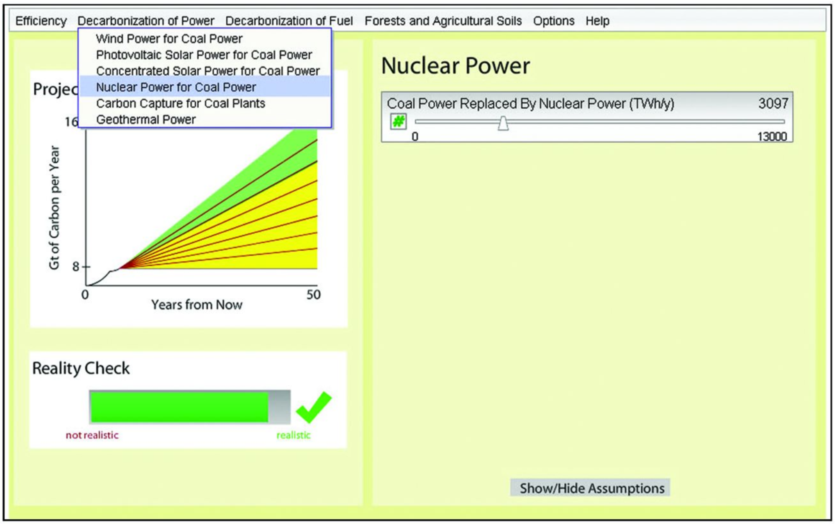

Figure 17. The interface for the applet Carbon Stabilization Wedges. (http://www.explainingclimatechange.ca/Climate%20Change/swf/Stabilization%20Wedges/stabilizationWedges.swf)

As an example, consider the replacement of thermoelectrically generated electrical energy with photovoltaic energy. A case study might be developed of a homeowner with an annual electrical energy consumption of 10 MWh wishing to install a 2.6 kW photovoltaic panel array on the roof of her home in Edmonton, Canada – a large northern city (53° N). Edmonton has on average 2300 bright sun hours per year. What fraction of her electrical energy can reasonably be "de-carbonized"? To estimate this, consider the annual power output from such an array. While the maximum power is 2.6 kW this only occurs at peak times (mid-summer) when insolation is at its maximum. When averaged over the entire year, 1.4 kW would be a better estimate of the power output. Thus, over 1 year the energy produced is

$$E_{solar} = (1.4\,kW)(2300\,h) = 3.2\,MWh$$

The cost of such an array is approximately $15K and if this is amortized over a 25 year period (typical warranty period for such systems) the cost of electrical energy is on the order of $0.19/kWh – which is the same magnitude as thermoelectrically produced electrical energy. As well the homeowner has de-carbonized her electrical energy by about 30%. 3.2 MWh of energy is, by unit conversion equivalent to 1.15×10^{10} J = 11.5 GJ of energy. Commonly published data indicates that coal is approximated 80% carbon and produces on average 24 MJ/kg when combusted. If a typical efficiency for thermoelectric power production is 30% then each kg of coal will produce 7.2 MJ of electrical energy. The homeowner has offset

$$\left(\frac{11.5\,GJ\,/\,a}{7.2\,MJ\,/\,kg}\right)\times 0.8 = 1278\,kg$$

or over 1 T of carbon. By itself this is a modest reduction of carbon emission. Clearly, stabilization of atmospheric carbon will not occur solely by switching to solar energy! The point of the Carbon Stabilization Wedges applet, however, is to demonstrate that many small, coordinated changes can lead to stabilizing carbon emissions into the atmosphere. An important benefit to students, aside from using scaling arguments to solve practical problems is to help them visualize solutions and see that our collective efforts can make a positive change to the problem of carbon loading in the atmosphere. Anthropogenic climate change is not an intractable problem.

The approach taken in the Carbon Stabilization Wedges simulation seems to resonate particularly well with the approach described by Sterman (*13*).

"Learning arises in the process of interacting with the models, hypothesizing how the system might respond to policies, being surprised, forming new hypotheses, testing these with new simulations and data from the real world."

A Sea of Change in How We Teach Science? Project and Rich Context Driven Science Teaching

We began this chapter by making the case that achieving climate literacy in light of public attitudes toward climate change is one of the most important challenges facing science educators in the 21st Century. The challenges arise for many reasons, including the complexity inherent in understanding our planetary boundaries; the multi-disciplinary approaches required to make sense of our changing climate; and the one-way transmission pedagogical models that still operate in many undergraduate classrooms. Much of the fundamental science underlying climate change falls into the domain of Chemistry and Physics education, yet overt connections to this important planetary context are not often made in undergraduate curriculum in these disciplines. Making sense of complex science does not lend itself well to strictly disciplinary approaches or to one way transmission pedagogical approaches. What is needed, instead, are more active learning approaches that engage learners in more interactive ways with evidence and allow them to construct their own mental models that are built upon fundamental science concepts. Yet the ready availability of resources that embed climate science principles in chemistry and physics learning outcomes and facilitate the construction of robust mental models is a substantial barrier to moving the bar toward greater climate literacy.

The seven exemplars of interactive simulations presented in the chapter are based on our understanding of best practices in the use of simulations and visualizations in addressing complexity. They have been developed to support a variety of active learning approaches, and to help students develop an evidential basis for climate science, while concurrently mastering fundamental understanding of chemistry and physics.

The dual challenge of visualizing the science of climate change while changing the climate of science teaching is daunting, but thoughtfully designed visualizations have an important contribution to make in meeting that challenge. After analyzing the difficulties of building mental models that adequately address complex dynamic systems such as climate and the economy, Sterman concludes (*16*) that simply providing more information is not a remedy, but new modes of communication are required, including experiential learning environments such as interactive simulations.

He concludes: *"When experimentation is impossible, when the consequences of our decisions unfold over decades and centuries, that is, for climate change and many of the important issues we face, simulation becomes the main—perhaps the only—way we can discover for ourselves how complex systems work, what the impact of different policies might be, and thus integrate science into decision making."*

The two sets of resources at www.explainingclimatechange.com and www.Vc3chem.com are freely available to instructors and students as a step toward achieving Sterman's goal.

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