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To appear in *Visualization in Science Education*, John Gilbert (Ed.)

Chapter 9

ASSESSING LEARNING FROM THE USE OF MULTIMEDIA CHEMICAL VISUALIZTION SOFTWARE

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Abstract: This chapter extends the use of cognitive and "situative" theories of learning described in our earlier chapter to discuss the design of five chemistry multimedia visualization projects. All five projects are shown to enhance the learning of chemistry concepts and development of scientific investigative process skills. Two projects emphasize the social processes associated with scientific investigation with bench laboratory components; two others without laboratory components could be easily utilized in ways that develop such social processes; and the fifth is shown to enhance visualization process skills although it was designed based upon the cognitive theory of multimedia learning. In order to assess the developing levels of visualization skills of novice chemistry students supported by all five visualization projects, non-traditional testing items must be utilized. Samples of several multimedia testing items addressing both conceptual and process skills are discussed and used in studies of the efficacy of the most cognitive-theory based project. A study using the project with the closest alignment to "situative" theory illustrates how the rubric for representational competence levels discussed in our earlier chapter is applied to show changes in visualization abilities of students. The chapter concludes with brief suggestions for future development of visualization software, visualization-based instructional activities and testing activities.

1. VISUALIZATIONS IN CHEMISTRY

In an earlier chapter (Kozma & Russell, this volume) we established the desirability for inclusion of chemistry curricular components specifically designed to address the acquisition of chemical visualization skills which we defined as representational competence. These skills include the ability to utilize chemical symbols, chemical equations, various types of structural diagrams, diverse graphical formats including spectral plots and computer models, and nanoscale animations as appropriate for solutions of problems or tasks and the investigation and understanding of phenomena and concepts. Two theoretical bases for development of visualization skills were discussed – cognitive and situative. Cognitive theory (Mayer, 2003, 2002, 2001) addresses the transformation of these external symbolic representations to internal mental representations – mental models. Situative theory (Greeno, 1998; Roth, 1998, 2001) focuses on learning science as an investigative process and the use of social discourse and representations to support this process. In the earlier chapter we showed that representational competence levels of novice students can be enhanced through classroom, laboratory, and individual use of molecular modeling and computer simulations and animations. In this chapter we extend this discussion to several multimedia chemical visualization software packages. We include packages with both cognitive and situative goals and shall assess their designs and efficacies from one or both perspectives. Critical to such analyses are the development of new assessment tools to probe visualization skills and students' abilities to apply such skills.

The goals of this chapter are:

- to review five multimedia chemical visualization packages with respect to their design characteristics and learning goals,
- to discuss special assessment tools and techniques useful for measuring visualization skill levels,
- to summarize some of our studies of the efficacy of our multimedia visualization programs, *Synchronized Multiple Visualizations of Chemistry* (*SMV:Chem*) (Russell, Kozma, Becker, & Susskind, 2000), and , *ChemSense* (Schank & Kozma, 2002) using these new assessment tools, and
- to suggest directions for future instructional improvements and research.

This chapter is divided into four major sections addressing each of these four goals. We include a sufficient number of black and white figures in the printed text to allow logical development of our goals without access to a computer or the Internet. However, on the accompanying CD-ROM we provide color versions of all figures, examples of all *SMV:Chem* experiments discussed in the text in a new web-based format, examples of *SMV:Chem*-based homework assignments in the web format, and an example of visualization skills assessment tools used in our study of the efficacy of *SMV:Chem* in classroom and out-of-class use. Whenever possible we provide URLs for viewing samples of the multimedia software packages.

2. MULTIMEDIA VISUALIZATION PROJECTS

A number of large-scale multimedia projects have been developed in the U.S., often with funding from the National Science Foundation, to use the capabilities of new technologies to improve chemistry instruction and learning. In this section we review several of the major projects and feature our project, *SMV:Chem*.

We use the two theoretical approaches described above—the cognitive and situative theories—as structural schema for analyzing these projects. Some projects explicitly cited one or the other of these theories in developing their software tools and instructional approaches; others did not. Nonetheless, it appears to us that some of these projects emphasize the learning of chemical concepts, principles, and procedures, while others emphasize the learning of the scientific process of chemical investigation. As we mentioned above, these two types of educational goals are not mutually exclusive; they can be complementary. Indeed some of these projects incorporate aspects of both. As multimedia projects, they also often incorporate several types of visualizations—models, simulations, and/or animations.

2.1 Synchronized Multiple Visualizations of Chemistry (SMV:Chem)

SMV:Chem is a chemical visualization software program designed to assist students to develop their abilities to use appropriate visualizations including nanoscale models and animations as well as various symbolic representations as they seek to understand and explain chemical concepts and solve chemical problems (Russell & Geno, 2000; Russell, 2004). Version 1.0 (MAC and Windows 95 & 98) was distributed in 2000-2002 by John Wiley & Sons (Russell, Kozma, Becker, & Susskind, 2000). Version 2.0 (MAC and Windows 2000, ME, XP, and NT) is available from the authors (russell@oakland.edu). A sample subset of the web-based Version 3.0 is included on the accompanying CD-ROM and can be accessed via the Internet at http://www2.oakland.edu/users/russell. *SMV:Chem* was based upon a prototype, *4M:Chem – MultiMedia and Mental Models in Chemistry* (Russell & Kozma, 1994; Russell, Kozma, Jones, Wykoff, Marx, & Davis, 1997).

SMV:Chem and *4M:Chem* were designed for use in the classroom to allow instructors to show examples of real experiments and ways to represent the experimental phenomena with molecular-scale animations, graphs, molecular models, and equations and for use by students outside the classroom to enhance their chemical visualization skills and conceptual understanding. A secondary classroom goal was to promote an interactive classroom environment that stimulated class discussion with the pace and directions of usage controlled by the instructor’s assessment of class responses. Both programs used a consistent screen design with experimental videos, nanoscale animations, graphical representations, and other representations such as chemical equations, text, data collection sheets, and molecular models in respective quadrants of the screen. All experiments discussed are included on the CD-ROM in the new web-based format.

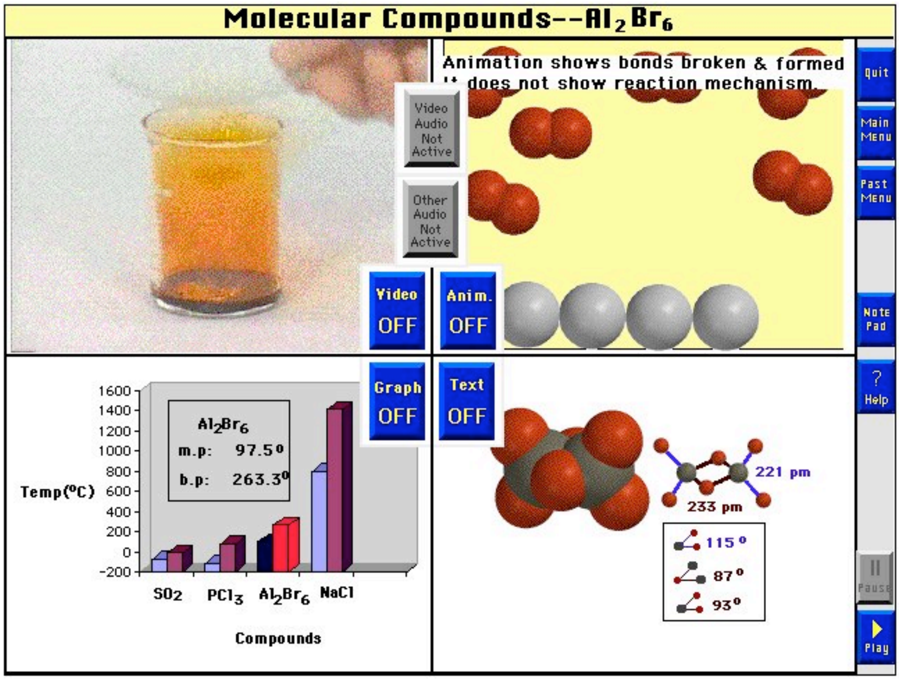
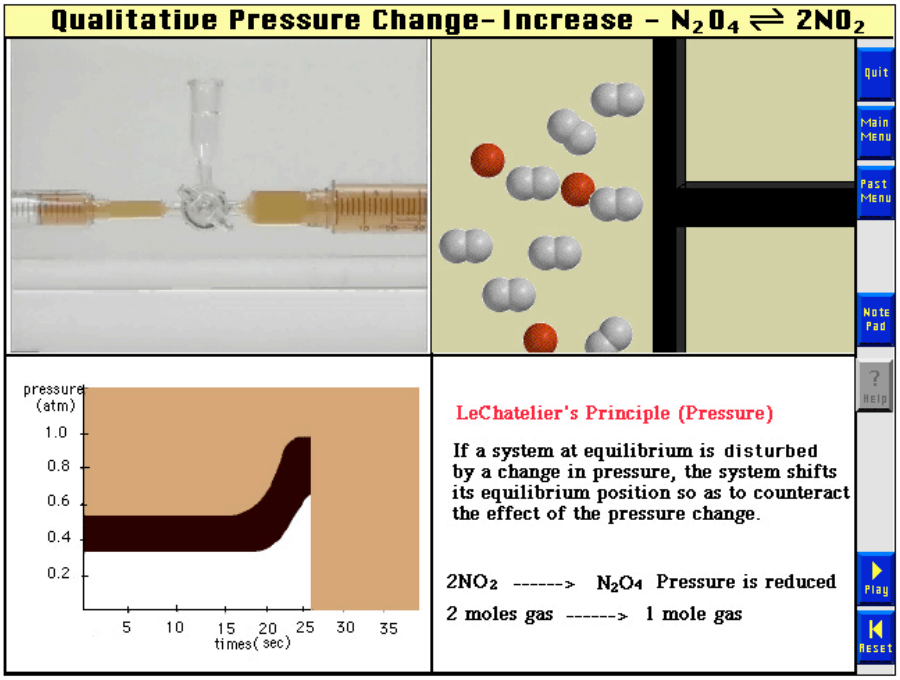

Animation shows bonds broken & formed
it does not show reaction mechanism.

Figure -1. Window selection and program control screen for a SMV:Chem experiment.

Once a specific experiment has been chosen a screen such as in Figure 1 appears to allow selection of one to four windows using the buttons at the center of the screen and program control using buttons on the right vertical toolbar. There are separate audio tracks for all windows that can be activated or deactivated. In Figure 1 the visualizations in the lower two windows are static although in most experiments the graphs are dynamic. Using the Pause/Play buttons windows can be frozen at any point and restarted.

The experiment depicted in Figure 2 shows the effect of decreasing the volume on an equilibrium mixture of two gases, $N_2O_4 \rightleftharpoons 2NO_2$. This particular example was selected since at room temperature a sample can be prepared with near equal amounts of both gases but only the NO_2 can be observed by the eye. The UV-visible absorption spectrum shows a broad absorption centered at 400 nm with its long wavelength tail extending to 650 nm giving the sample a red-brown color. N_2O_4 has a sharper absorption band at 335 nm which does not extend past 400 nm making it invisible to the human eye.



Qualitative Pressure Change- Increase - $N_2O_4 \rightleftharpoons 2NO_2$

LeChatelier's Principle (Pressure)

If a system at equilibrium is disturbed by a change in pressure, the system shifts its equilibrium position so as to counteract the effect of the pressure change.

$2NO_2$ ------> N_2O_4 Pressure is reduced

2 moles gas ------> 1 mole gas

Figure -2. SMV:Chem screen for LeChatelier's principle experiment showing effect of a change in volume on the equilibrium compositions of the sample. Viewed on the computer screen the color of the gas in the 1 cm square tube left of the stopcock is definitely lighter than the color in the gas in the 2 cm square tube right of the stopcock.

Users are encouraged to view first only the video window and to replay the experiment until they have a through understanding of how the experiment shows a change in equilibrium composition that produces more N_2O_4 resulting from decreasing the volume. At the start of the video the three-way stopcock is positioned 45^0 counterclockwise from its position in Figure 2 such that there is an open path between the two sides of the apparatus. The stopcock is rotated clockwise to the position shown which isolates the two sides. At this point the partial pressures of NO_2 are the same in both the left 1.00 cm square tube and the right 2.00 cm square tube. The sample appears darker on the right since there are twice as many NO_2 molecules in the viewing path as you look through the tube. The left syringe is pushed in until reaching the point where the volume in the isolated left side is exactly half its initial volume. If there was no change in the equilibrium composition, by Boyle's law the partial pressure of NO_2 would have doubled. With double the pressure and half the path length the color of NO_2 gas on both sides should be identical. The observation that after this change in volume the color on the left is lighter than the color on the right shows the composition has shifted to produce more colorless N_2O_4 leaving less red-brown NO_2.

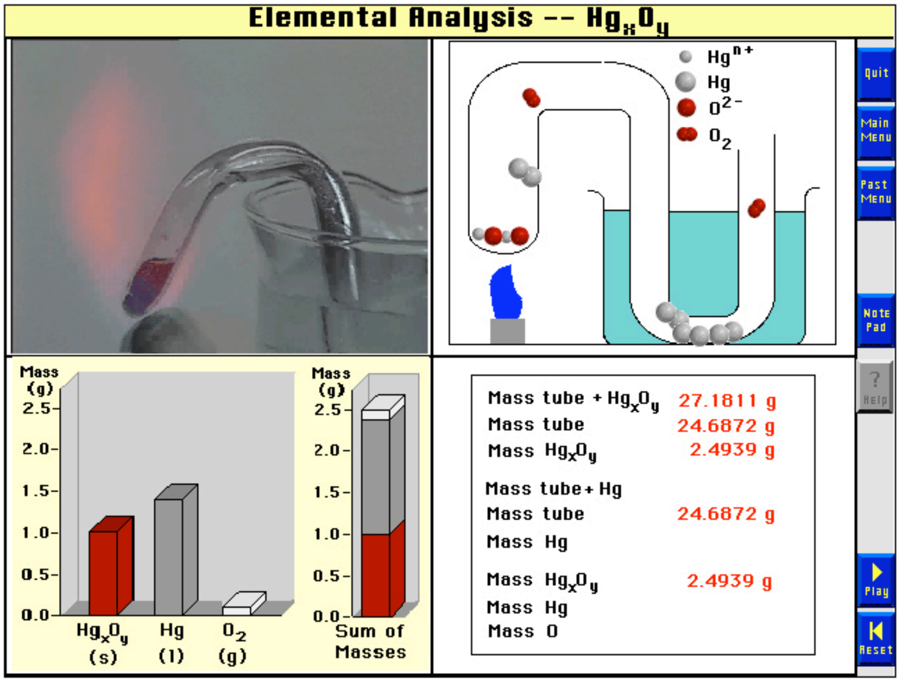
If the experiment is rerun activating both the video and animation windows, the animation shows initially five red-brown spheres and seven coupled gray spheres all in constant motion. Prior to the piston moving in from the right to cut the volume (area) in half the distribution of species is seen to alternate between five red-brown monomers/seven gray dimers and seven monomers/six dimers as the dimers decompose and the monomers dimerize showing the dynamic property of a chemical equilibrium. After the volume was cut in half, the animation shows the composition alternating between three monomers/nine dimers and one monomer/ten dimers.

Class discussion or homework questions might ask students to consider what is shown in the animation that is not visible in the video of the experiment, which properties of a chemical equilibrium are correctly and which incorrectly shown by the animation, and how LeChatelier's principle could be used to explain the observed and portrayed shift in composition. The animation shows the dimers that form upon reaction of two monomers even though these species represent the unseen colorless N_2O_4 molecules. The animation correctly shows the dynamic properties of a chemical equilibrium but shows a fluctuation in composition where equilibrium compositions are constant. This discrepancy is usually quickly attributed by students to the small numbers of species shown in this animation. The increase in pressure produced by the decrease in volume can be partially offset by forming more N_2O_4 since such formation reduces the total number of gas molecules present in the sample. On rare occasions some student will note that the shift in composition in the animation appears very dramatic while that in the video was barely visible. This is a perfect lead-in to viewing the graphical representation which is quantitative rather than qualitative as the animation. After discussing the graph instructors can show the video, animation, and graph simultaneously and ask if the equilibrium shift could be accurately portrayed by the animation and how many molecules would be required.

Animations used for the eleven *SMV:Chem* gas equilibrium experiments with NO_2 and N_2O_4 all use animations with red-brown spheres for NO_2 and coupled gray spheres for N_2O_4. This choice of models rather than use of space filling models of these molecules with the usual color coding for atoms with blue for N and red for O is consistent with the adaptation of Mayer's Coherence Principle to visual objects (See Mayer 2001, 2002 and the discussion of cognitive theory in the previous chapter). This principle states that extraneous objects should be excluded. The primary point to all equilibrium animations is to show the dynamic property of chemical equilibria. We did do a pilot test using the red-blue space filling models for these molecules. In that case reactants and products could only be distinguished by their shapes. When asked to view animations using both types of models no students noticed the dimerization and dissociation reactions occurring with the space filling models but many made this observation with the red-brown spheres and gray coupled spheres.

In designing the animation and graphical representations we took advantage of color to connect species with the two gases, brown for NO_2 and light gray for N_2O_4. Our earlier work showed that most students first use surface features of representations to answer questions concerning all types of visualizations. Color was shown to be a most important property when comparing two visualizations. The sample used in this experiment was initially 38% NO_2 and after the volume was cut in half became 28% NO_2. The experiment in Figure 2 has been paused just as the final volume was reached and the new final equilibrium established. At the end of the experiment the 28% and 38% figures are added to the graph as are two lines to show where the two vertical boundaries of the brown NO_2 band would have been with no shift in equilibrium composition.

Figure 3 shows a screen capture for another *SMV:Chem* experiment designed to allow the determination of an empirical formula. A glass tube of the shape shown in the animation window is weighed, a sample of red mercury(II) oxide added, and the tube and solid weighed. The tube is clamped with its U-bend in a water-ice bath and the closed end with the red solid heated. Upon heating the amount of solid decreases and droplets of liquid mercury are observed to form in the tube. Once the solid at the end of the tube has disappeared the tube is removed form the bath, dried, and weighed. When used in class or for homework this experiment is first run with the video and text windows active. As mass measurements are made the resulting data is entered into the table shown in the text window.



Mass tube + Hg_xO_y 27.1811 g
Mass tube 24.6872 g
Mass Hg_xO_y 2.4939 g
Mass tube + Hg
Mass tube 24.6872 g
Mass Hg
Mass Hg_xO_y 2.4939 g
Mass Hg
Mass O

Figure -3. SMV:Chem screen from experiment to determine the empirical formula of a red mercury oxygen compound.

The animation for this experiment includes both models of nanoscale species (Hg atoms, O_2 molecules, and Hg^{2+} and O^{2-} ions) and macroscopic objects (sample tube, water-ice bath, and Bunsen burner). During meetings of the advisory board for the *4M:Chem* prototype project when shown animations mixing objects of such difference size scales in a diagram the science educators were concerned that would promote or reinforce students' misconceptions. All board members who were scientists thought that it was obvious the intent and students would not be confused. Over the years that we have used such animations no student has questioned in class or indicated on homework that he/she did not recognize the scale differences of the components of the animation. In fact, we have used this animation to discuss the distinction between nanoscale representations of chemical phenomena and macroscopic observations. The mercury ion's legend on the animation is shown with unknown charge since the primary objective of the experiment was to find the empirical formula of the red solid. Although the animation does start with equal numbers of mercury and oxygen ions thus signifying an HgO empirical formula, you can count on students to use numbers wherever available and to determine the empirical formula from the numeric data rather than by simple examination of the animation.

The graphical representation for this experiment is rich in data and allows discussion in class or questions on homework of many topics. For example, the experiment could be paused at the position shown in Figure 3 and the class asked what would be the weight of the sample in the tube at that point if it were removed from the bath and dried and if the empirical formula could be determined with this data. Other potential questions are – What does the right graph show? How will the right graph appear at the end of the experiment (students have already seen the video of the experiment)? How does the graph show conservation of mass? This last question is, of course, another version of the first question that provides the concept but does not direct attention to the right graph. When observed on the computer screen you would note the use of silver or gray to represent mercury in the animation and graph, the use of white in the graph to represent the colorless oxygen gas released into the atmosphere, and the red color in the graph to show the original red solid.

The final data shows there were 2.3112 g of Hg and 0.1827 g of O in the original 2.4939 g of the red solid. This data corresponds to 0.011522 moles of Hg and 0.01142 moles of O clearly giving an empirical formula of HgO. Using the data in this experiment, students could be asked to find the theoretical and percent yield of Hg knowing the empirical formula is HgO. They would get 2.3097 g theoretical yield and 100.06 percent yield. If asked to explain how they could get a percent yield above 100%, the most common responses are that there are impurities in the sample or the tube was not dry. Seldom do students respond that within the experimental uncertainty 100.06 is 100%. It is worth noting that these data, as all data in the *SMV:Chem* experiments, were those recorded in the laboratory as the experiments were filmed. No video results were adjusted to give "good" data.

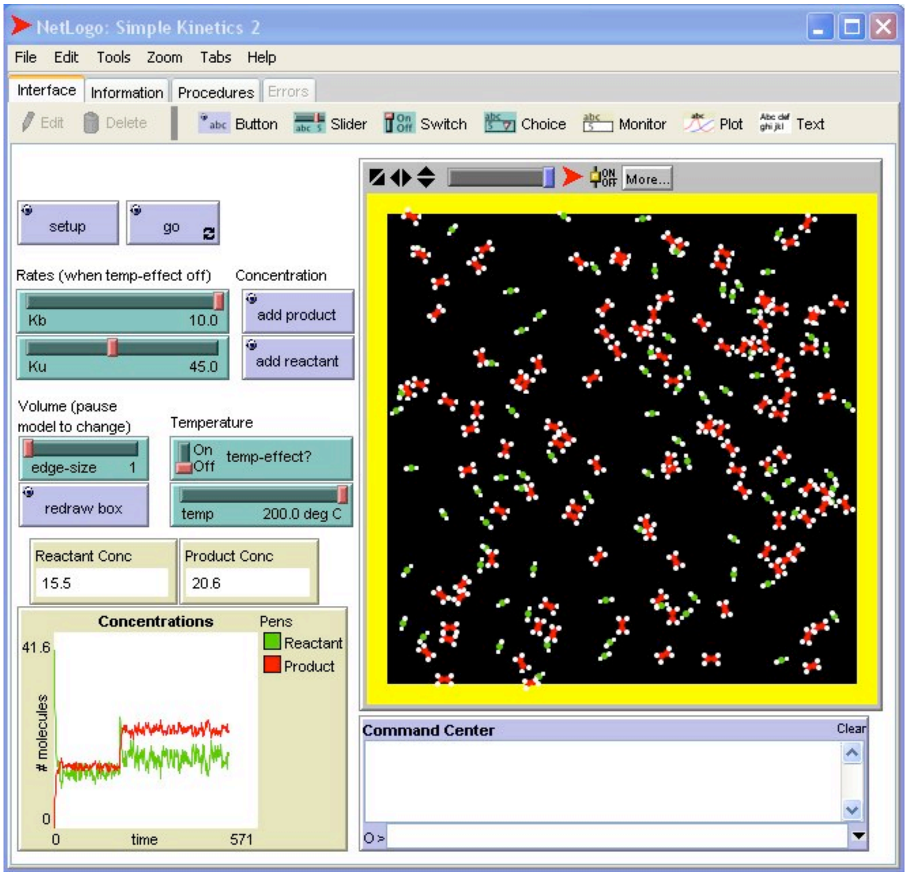
We have made use of audio tracks throughout *SMV:Chem* experiments consistent with Mayer's principles of multimedia learning. Using the audio option the software satisfies the multimedia principle of using words and pictures and the Contiguity, Modality, and Redundancy Principles of using words and picture simultaneously without repeating the words in an on-screen text. The style of the narration is conversational rather than a more formal scientific style thus satisfying the Personalization Principle. We address the Interactivity Principle by providing buttons that allows students conveniently to pause, restart, and replay experiments and to select visualization viewing combinations from single, all possible duets and triplets, to all four windows.

Although *SMV:Chem* was designed to help students gain deeper understanding of basic chemical concepts and phenomena, its use of alternative nanoscale and symbolic representations was also designed to promote student use of such representations when solving chemical problems or considering chemical phenomena. Attainment of the cognitive goals as noted above is supported through consideration of Mayer's guidelines for multimedia instruction. In the assessment section below we show sample questions that measure attainment of both deeper conceptual understanding and abilities to utilize alternative forms of representations to understand chemical phenomena – process skills characteristic of investigative science encompassed by situative theory.

2.2 Connected Chemistry

Like *SMV:Chem*, *Connected Chemistry* is an example of a multimedia project that is targeting the learning of difficult chemistry concepts (Stieff & Wilensky, 2003). The software is a collection of computer-based simulations of closed chemical systems that students can interact with in several ways. Each simulation focuses on a chemical concept such as factors effecting rates of reaction or LeChatelier's principle. *Connected Chemistry* is written in NetLogo, a multi-agent modeling language. The interface window of *Connected Chemistry* for the "Simple Kinetic 2" module is shown in Figure 4. The interface consists of three fundamental components: a graphics window for a nanoscale representation of the system, a plotting window for graphs of macroscopic properties of the system, and an area for setting system parameters and starting, pausing, restarting, and resetting the simulation.

This module in Figure 4 simulates the equilibrium, $2\ NO_2(g) \rightleftharpoons N_2O_4(g)$, and is designed to explore LeChatelier's principle. The graphics window displays visualizations for two types of molecules, a three atom linear molecule shown on the computer screen as white-green-white circles and a six atom molecule visualized with two central red circles and two white circles attached to each red circle representing NO_2 and N_2O_4 respectively. (Note: these models do not reflect the geometric structures of bent NO_2 and N_2O_4 whose lowest energy structure has mutually perpendicular NO_2 groups.) Unless the user pauses the simulation, all molecules in the graphics window are in rapid motion. The plotting window shows the number of reactants, NO_2, and products, N_2O_4, versus time. The graph for the number of N_2O_4 product molecules is shown in red corresponding to the red color used for the nitrogen atoms in the N_2O_4 models in the graphic window. The color green is used for the NO_2 graph in the plotting window and nitrogen atoms in the NO_2 models in the graphics window. The use of red and green for nitrogen atoms in the N_2O_4 and NO_2 models in the graphics window allows a quick visual estimate of relative numbers of these species once the simulation is paused. Note in the figure in the text the difficultly in making such an estimate based on model shapes since the red and green colors appear the same in the black and white print.



Kb 10.0

Ku 45.0

edge-size 1

On/Off temp-effect?

temp 200.0 deg C

Reactant Conc 15.5

Product Conc 20.6

Figure -4. Connected Chemistry interface window for Simple Kinetics 2 module. http://ccl.northwestern.edu.

For the conditions of this particular simulation the user chose to have initially only reactants present. The reactant numbers rapidly dropped and product numbers increased until they were fluctuating with about equal numbers of each as shown by the first horizontal region of the graph in the plotting window. At this point the user stopped the simulation and added extra NO_2 molecules causing the spike in the plot. Once the user restarted the simulation, reactant numbers dropped but leveled off at a new equilibrium higher than the old one. The product numbers increased but reached equilibrium at a higher value than the new reactant equilibrium value. This shows the LeChatelier's principle effect for changing concentration. The boxes at the top of the plotting window show the numbers of reactant and products at any time. These numbers are for some arbitrary volume to signify a concentration rather than the actual number of molecules shown in the two dimensional graphics area.

The system parameter area contains three sliders to set values for the forward rate constant, K_b, the reverse rate constant, K_u, and the temperature. Three other variables can be adjusted to add reactants, add products, and make the box smaller by making its walls thicker. The "setup" box is used to reset the graphic and plotting windows for the initial conditions selected for system parameters. Clicking the "go" box starts, pauses, and restarts the simulation. The tabs above the top tool bar open an "information" window and a "procedures" window. The information window contains a description of the chemical concept behind the model and suggestions on how students may wish to modify the model. The procedures window shows the programming code for the model which students can modify to test different models.

Stieff and Wilensky give six examples of use of *Connected Chemistry* in structured interviews with academically-talented upper division science majors that show them confronting and changing former misconceptions of LeChatelier's principle. A primary advantage of this software is the ease with which changes can be made in a wide range of system parameters and the consequences of each change rapidly observed. This should be most advantageous for instructors to the classroom where they can use the software to confront students' misconceptions. For example the effect of increasing the reactant concentration on a system at equilibrium shown in Figure 4 is obvious since the initial equilibrium had equal amounts of reactants and products. This initial equilibrium condition was achieved by adjustment of the relative values of K_b and K_u. Experienced instructors will recognize the experimental conditions that best show specific results that confront misconceptions or most obviously show the concept under discussion. For *Connected Chemistry* to be effective with less academically-talented students and high school or first year college students, we speculate these students will need a well designed guided inquiry approach whether in the classroom or for out-of-class assignments.

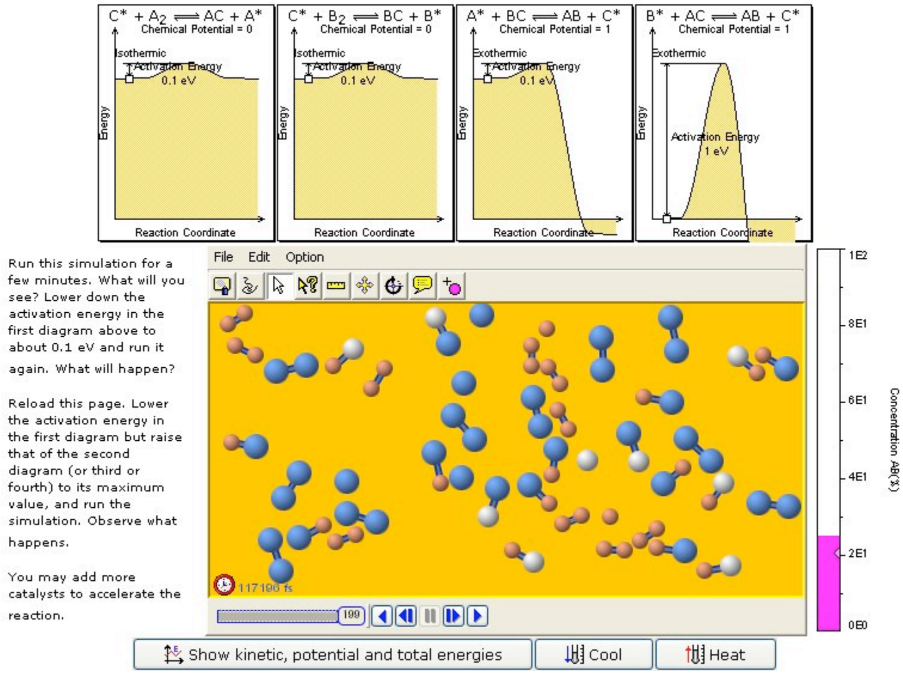
In an effort to make the simulation as close to reality as possible and take advantage of NetLogo's ability to show rule-driven motions of hundreds of objects, when the simulation is running the graphics window is a blur of motion. The slider above the graphics window allows the speed of the simulation to be reduced. Only when the simulation is paused can features of any molecules be observed and then there are so many objects that only crude conclusions can be drawn such as there appears to be many more product molecules than reactant molecules. All quantitative conclusions from this simulation are derived from the graph in the plotting window and the counters for concentrations. The nanoscale display in the graphics window should help students tie the observable macroscopic properties shown in the plotting window to the underlying molecular behavior and is probably the focal point for student attention. The option for students to modify the code and test alternative models available in *Connected Chemistry* is likely to be seldom used due to time constraints on both students and instructors.

Analyzing *Connected Chemistry* using cognitive theory and Mayer's principles of multimedia instruction, it comes out very high on the Interactivity Principle, if that principle is expanded to control more than rates of presentation. The absence of audio and restriction of words to a minor role in the separate information window take the other eight principles outside the realm of the software and rely on the instructor's verbal narration. This supports our conclusion stated above that *Connected Chemistry* requires a skilled instructor and a well-designed guided inquiry organization when implementing the module.

Connected Chemistry allows users to plan experiments to test various hypotheses or to simply explore the results of variations of several experimental parameters in an attempt to formulate hypotheses and to use the simulation to quickly see the results. In this light, users are learning chemistry in a true investigative mode and on a time scale much compressed from what would be required with hands-on laboratory experiments. In order for *Connected Chemistry* to be more aligned with situative theory, it would have to engage students in the investigation of real chemical phenomena and the social processes associated with these investigations.

2.3 Molecular Workbench

As with *Connected Chemistry*, the goal of *Molecular Workbench* is to use advanced computational techniques and visualizations to help students develop appropriate mental models of different chemical systems and concepts. *Molecular Workbench* provides a variety of real-time, interactive simulations of chemical phenomena by adding sets of rules describing chemical reactions to a molecular dynamics modeling system (Xie & Tinker, in press). Simulations for a wide variety of topics are available at http://workbench.concord.org/modeler/index.html. All simulations are calculated and displayed for a two-dimensional molecular dynamics model with the potential energy for forming molecules at 0 K taken as the sum of electronic energies for each bond and adjacent pair of bonds with the total potential energy the sum of two- and three- center terms. Added to the potential energy are terms for intermolecular forces for van der Waals, electrostatic, bond stretching, and bond angle bending. Motions of all species in the simulation are calculated with Newton's equations of motion with the parameterized potentials. To account for chemical reactivity at each step in the simulation the energy of each bond is compared with a table of energies required to break particular bonds and the energies of nearby unbound atoms to determine if a bond could form as discussed in the example below. The software has the flexibility to allow users to set most initial parameters including the atoms, their positions, velocities, and bonds as well as all potential energies parameters. To simplify use, an initial simulation with preset values for these parameters is provided for each topic. Many topics allow users to add or subtract thermal energy and rerun the simulations.



Run this simulation for a few minutes. What will you see? Lower down the activation energy in the first diagram above to about 0.1 eV and run it again. What will happen?

Reload this page. Lower the activation energy in the first diagram but raise that of the second diagram (or third or fourth) to its maximum value, and run the simulation. Observe what happens.

You may add more catalysts to accelerate the reaction.

Figure -5. Molecular Workbench simulation of homogeneous catalysis for $A_2 + B_2$ _ 2 AB with catalyst C. Models: A – small dark sphere, B – large dark sphere, C – intermediate light sphere

As an example of one *Molecular Workbench* simulation, Figure 5 shows a snapshot of the computer screen as the simulation progresses for a homogeneous catalysis. This screen is for the catalyzed mechanism:

$C + A_2$ _ $CA + A^*$ (1)

$C + B_2$ _ $CB + B^*$ (2)

$A^* + CB$ _ $AB + C$ (3)

$B^* + CA$ _ $AB + C$ (4)

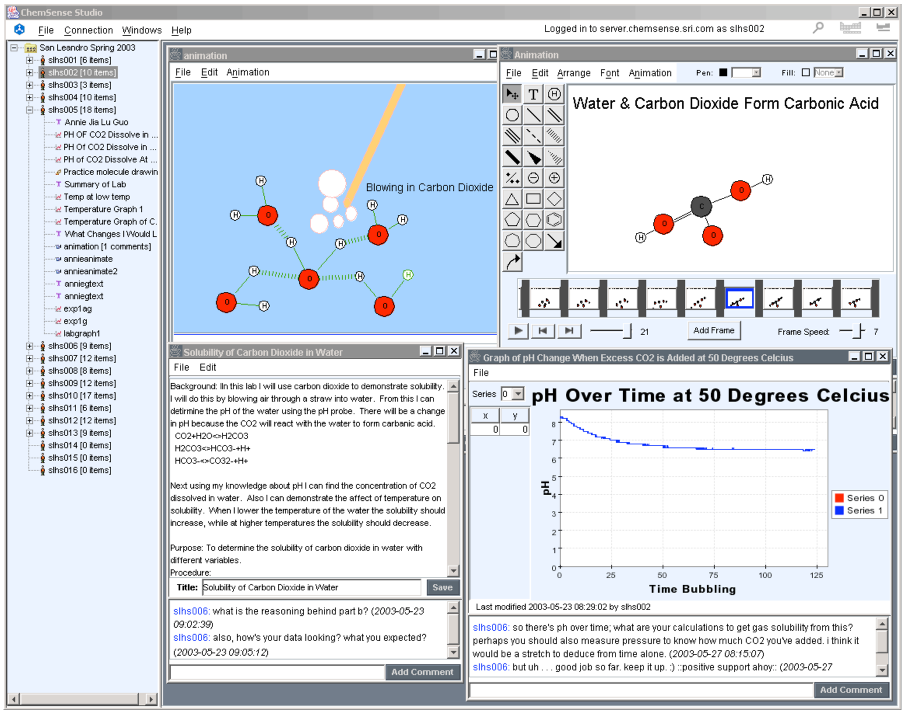
To simulate this mechanism the activation energies of the dissociations of A_2 and B_2 and for the reactions $A^* + B_2$ and $B^* + A_2$ are set high so they will not occur at the temperature of the simulation. The screen in Figure 5 shows that five parameters can be easily adjusted – the four activation energies by moving the square at the end of the arrows for the activation energies up or down on the four energy diagrams at the top of the figure and the temperature using the cool and heat buttons at the bottom of the figure. In the particular simulation shown in Figure 5 the activation energy for step (4) was made high cutting off this step. Note at the point of the simulation shown the product AB was formed by step (3) and every species shown in this mechanism is present. Observation of the simulation shows that CA and CB molecules do dissociate upon some collisions with other molecules. If CA molecules did not dissociate, then CA would accumulate since step (4) is not possible. The reaction would proceed until all C was bound in CA. This end state could be formed by lowering the temperature such that collisions of CA molecules don't have enough energy to break the CA bond. The original simulation for this topic shown on a prior screen had the activation energies for all four of these steps set low such that the reaction proceeds to give only AB and free catalyst C since the numbers of A_2 and B_2 were initially equal.

An initial study of *Molecular Workbench* found that it did support student understanding. Pallant and Tinker (2004) found that when students used *Molecular Workbench* they accurately recalled arrangements of the different states of matter, and could reason about atomic interactions. These results were independent of gender and they held for a number of different classroom contexts. Additionally, a close evaluation of students' responses about the bulk properties of atoms and molecules revealed that many fewer students had misconceptions following the intervention as compared to their responses on the pre-test. Follow-up interviews indicated that students were able to transfer their understanding of phases of matter to new contexts, suggesting that the knowledge they had acquired was robust. Xie and Tinker (2004) claim their work with other simulation systems (Pallant & Tinker, 2004) indicates maximum learning occurs when students experiment with the simulations with some instructor guidance. Instructors might ask students to determine if products will form if any one of the four activation energies is set to its upper limit with the other three set low, perform the simulations and explain what they observe. Instructors could follow-up by asking students to predict if they expect the same results at high and low temperatures, to try those experiments, and explain the results.

Just as with *Connected Chemistry*, *Molecular Workbench* scores high on the Mayer Interactivity Principle but the other Mayer multimedia instruction principles do not apply due to the lack of audio tracks. *Molecular Workbench* simulations promote investigative science learning. The catalysis example in Figure 5 allows users to explore five parameters associated with the proposed mechanism and rapidly observe results of changes in any of these parameters. This catalysis simulation is much more sophisticated than the states of matter simulations used in the Pallant and Tinker (2004) study noted above. If maximum learning using the states of matter simulation required instructor guidance, a more directed guided inquiry approach would likely be needed for students to understand the full consequences of various relative activation energies for the four steps in the proposed mechanism. This example does allow students to explore the mechanism in ways impossible in the laboratory since each simple change in any activation energy would mean use of a different catalyst. This point should be made specific by the instructor as well as noting the assumptions about the reactivities of A_2, B_2, and AB with other species implicit in this four step mechanism. As with *Connected Chemistry*, *Molecular Workbench* would have to connect these simulations with the physical and social processes of scientific investigation if it were to be strongly aligned with situative theory.

2.4 ChemSense

While *Connected Chemistry* and *Molecular Workbench* support student learning of chemical concepts and principles, *ChemSense* is designed to support student inquiry in the wet lab. The *ChemSense* environment offers an ensemble of tools that enable students to create their own representations of chemical phenomena (Schank & Kozma, 2002). The basic premise of the *ChemSense* design is that these tools will be used within a social context (students collaboratively create representations) to investigate, analyze, and discuss chemical phenomena (students conducting wet lab experiments). Students use the tools in the *ChemSense* to express their chemical understanding in a jointly shared representational space and do this within a classroom and task context which includes physical lab equipment and data collection probeware.



Background: lIn this lab I will use carbon dioxide to demonstrate solubility. I will do this by blowing air through a straw into water. From this I can detirmine the pH of the water using the pH probe. There will be a change in pH because the CO2 will react with the water to form carbanic acid.

CO2+H2O<>H2CO3
H2CO3<>HCO3-+H+
HCO3-<>CO32-+H+

Next using my knowledge about pH I can find the concentration of CO2 dissolved in water. Also I can demonstrate the affect of temperature on solubility. When I lower the temperature of the water the solubility should increase, while at higher temperatures the solubility should decrease.

Purpose: To determine the solubility of carbon dioxide in water with different variables.
Procedure:

Title: Solubility of Carbon Dioxide in Water

slhs006: what is the reasoning behind part b? (*2003-05-23 09:02:39*)
slhs006: also, how's your data looking? what you expected? (*2003-05-23 09:05:12*)

Last modified 2003-05-23 08:29:02 by slhs002

slhs006: so there's ph over time; what are your calculations to get gas solubility from this? perhaps you should also measure pressure to know how much CO2 you've added. i think it would be a stretch to deduce from time alone. (*2003-05-27 08:15:07*)
slhs006: but uh . . . good job so far. keep it up. :) ::positive support ahoy:: (*2003-05-27*

Figure -6. The ChemSense screen for work by high school students. Upper left shows picture students drew to depict experiment of exhaling breath through a straw into water with pH initially adjusted to > 8.0. Upper right shows frame in student animation showing formation of H_2CO_3 and its partial ionization to H^+ and HCO_3^-. Graph is pH measured with pH probe showing formation of acidic solution as CO_2 dissolves in water.

Figure 6 shows the basic layout of *ChemSense*. The environment contains a set of tools – drawing, animation, graphing, and text tools – for creating and viewing representations, and a commenting feature for peer review. A web interface, called the *ChemSense Gallery*, is also available for viewing and commenting on work, and managing groups and accounts. Several examples of student-generated items can be seen in Figure 6. At the top of the window are two animations that students created to show the process of a gas – specifically, carbon dioxide – dissolving in water. To create these animations, students constructed individual frames that stepped through the breaking of bonds between the carbon, oxygen, and hydrogen, and the subsequent formation of carbonic acid, H_2CO_3 (aq). Below and to the right of the animations is a display of a dynamic graph that shows student-collected data from an experiment on the change in pH of the solution as carbon dioxide is dissolved over time. This data was collected at the lab bench through the use of probeware (developed by Pasco Inc., Roseville, CA) and imported into *ChemSense*. Below the graph is a comment area where other students can submit and view comments and questions. (Every item in the workspace has its own personal comment area.) To the left of the graph is a student-constructed description of the lab purpose, procedure, and findings.

In its use, *ChemSense* is designed to shape the way students think and talk while using representations to describe, explain, and argue about physical phenomena in terms of underlying chemical entities and processes. For example, in considering the dissolving of carbon dioxide into water, students can use the animation tool to build a representation of this dynamic process. As they create their animation they are confronted with a set of decisions about how to represent their understanding of the dissolving process – What does a carbon dioxide molecule look like? What is the structure of carbonic acid? What happens to the water and carbon dioxide structures as they meet? Which atoms are involved? How many are there of each kind? Discussions related to these decisions can engage students in the deep understanding of chemical phenomena in terms of underlying molecular structures and processes.

The *ChemSense* environment also gives students the means to coordinate these representations with observable phenomena using Probeware. Probeware allows students to directly import graphical or tabular data into their representations from bench top investigations and other inquiry-based activities (Krajcik et al., 1998; Roth & Bowen, 1999). For example, students collect wet-lab data such as temperature or dissolved oxygen content and import the data into *ChemSense*. They are then able to create and run two representations – a nanoscopic level representation showing the underlying process, and a tool-generated representation showing the change in observable properties. The goal of using two representations that show parallel changes at the nanoscopic and physical levels is to get students to question what is happening at the nanoscale that determines the emergent properties of what they see on the lab bench.

ChemSense is used in the context of specially designed curriculum units and investigative activities that scaffold student use of interconnected forms of visual and discursive representations and ask students to describe, explain, and argue about the chemical experiments they are conducting on the lab bench. In addition,, the environment allows students to peer-review each other's work by way of commentary. For example, a teacher may include as part of an activity a section towards the end of a unit that asks students to "review the work of two other lab groups and ask two questions related to the chemistry in their representation." As part of their "assignment", each lab group is responsible for providing critical feedback on other students' work.

Used appropriately, this function further supports the possibility for students to collectively arrive at new understandings of scientific concepts by asking students to probe other students' thinking (Bell & Linn, 2000; Brown & Campione, 1996; Greeno, 1998; Kozma, 2000a; Linn, Bell, & Hsi, 1998; Pea, 1992, 1994; Scardamalia & Bereiter, 1994).

Analyzed from a situative perspective, *ChemSense* supports students as they engage in investigations and use visualizations while working with each other to understand the chemical phenomena they are observing in terms of their underlying molecular structures and processes. As with *Connected Chemistry and Molecular* Workbench, ChemSense relies heavily on the skill of the teacher to structure the laboratory as an inquiry experience and to organize the class as a knowledge-building community. An observational study of students using *ChemSense* (Schank & Kozma, 2002) illustrating how the software can help students incorporate visualizations into their investigations and deliberations over their findings is discussed below.

2.5 ChemDiscovery

Like *ChemSense*, *ChemDiscovery* (formerly called *ChemQuest*) also supports chemistry inquiry. *ChemDiscovery* provides a technology-based, inquiry-oriented learning environment (Agapova, Jones, Ushakov, Ratcliffe, & Martin, 2002). Rather than using lectures and worksheets as the primary instructional vehicles, *ChemDiscovery* features interactive web pages linked to activities, databases, and design studios and coordinates with hands-on laboratory activities. Students work in pairs or small cooperative learning teams with instructors functioning most of the time as coordinators and facilitators rather than as spigots for knowledge. Agapova et al. list the following set of synergistic learning strategies that comprise the instructional philosophy of *ChemDiscovery*:

- Approaching content with relevant contexts
- Visualizing and modeling the molecular level of matter
- Engaging in inquiry through authentic science and design activities
- Discovering knowledge in a step-by-step manner
- Learning independently and in cooperative learning groups
- Self-constructed meaningful learning (from computer feedback to problem-solving and problem-constructing strategies
- Accepting responsibility for the environment
- Designing individual learning pathways through the course

ChemDiscovery consists of eight projects (i.e., quests) that can be used individually to supplement a traditional classroom or as a set to replace most of the traditional curriculum. These quests include topics such as design elemental substances, design chemical reactions between elements, and design and explore chemical systems. There are three entry points for each project: a set of learning goals for project activities or two contextual motivational tools introducing the project from environmental, scientific, and social perspectives. Each project includes design activities such as those shown in Figures 7 and 8.

After completing the design studio in which they design an atom of carbon (Figure 7), student teams construct a chemical reaction for formation of CO_2 from its elements as shown in Figure 8. They then build models of the molecules. A typical *ChemDiscovery* classroom would have student teams working simultaneously on a range of activities, either using computers for such activities as using design studios and extracting information from databases, performing hands-on laboratories, or working on designing strategies for problem solving. The multiple paths from initiation to completion of each project allow students to benefit from actions of their team as well as the others and to use learning activities and approaches suitable for varying abilities and interests. Students seek the knowledge and information to complete their activities, as needed. The goal is for students to gain a better understanding of chemical concepts and principles through investigation and accept greater responsibility for their own learning.

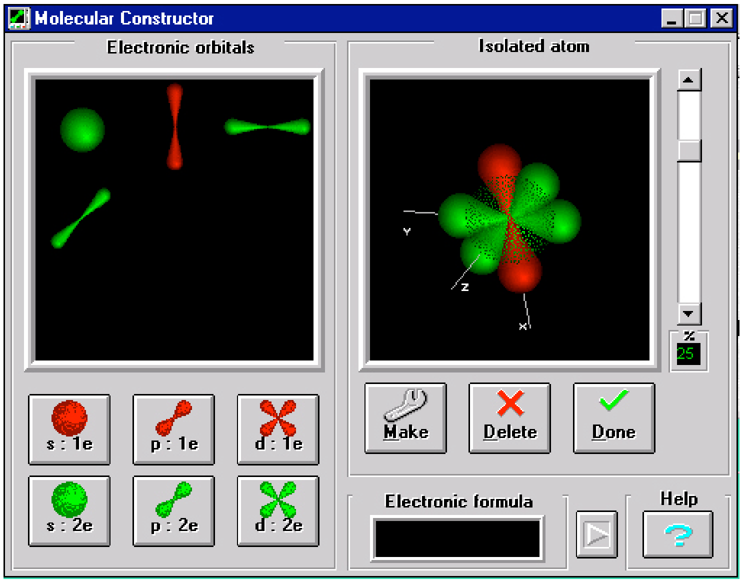
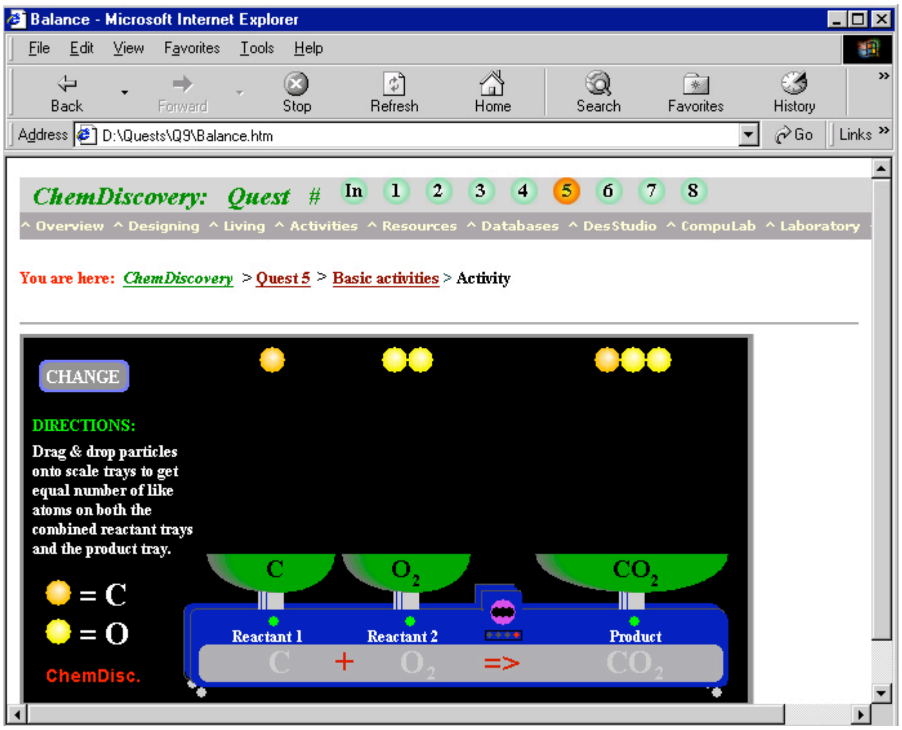


Figure -7. ChemDiscovery design studio for construction of an atom from atomic orbitals.



Drag & drop particles onto scale trays to get equal number of like atoms on both the combined reactant trays and the product tray.

Figure -8. ChemDiscovery design studio to model a chemical reaction between elements.

A team of researchers observed teachers using *ChemDiscovery* to varying degrees in a number of classrooms. Use of *ChemDiscovery* shifted the classroom focus as intended from a teacher-led lecture format to student-teacher interactions. Two teachers both taught different sections of their classes using *ChemDiscovery* and traditional instruction. They were observed to spend 38% of their time facilitating independent study work in their *ChemDiscovery* classes compared to 13% in their traditional classes. Journal entries of these teachers noted that students using *ChemDiscovery* had become more successful learners – connected new knowledge to prior knowledge, organized and reviewed new knowledge, and monitored their own understanding.

Although *Connected Chemistry*, *Molecular Workbench*, *ChemSense*, and *ChemDiscovery* all focus on chemistry as an investigational process rather than chemistry as a set of key concepts, *ChemSense* and *ChemDiscovery* include laboratory activities. Activities, such as working in cooperative teams, designing chemical systems, and analyzing extensive databases, engage students in challenging authentic scientific activities.

ChemDiscovery supports a situative approach to learning with focus on the physical and social characteristics of the environment. However, as with *ChemSense*, implementation of the situative approach with this project relies upon skilled instructors to guide student teams through the quests, structure their use of representation to support understanding, and make the quests authentic inquiry experiences. .

3. ASSESSMENT OF VISUALIZATION SKILLS

Williamson and Abraham (1995) in their study of the efficacy of computer animations showing nanoscale representations of chemical phenomena used a specially designed assessment tool called the Particulate Nature of Matter Evaluation Test (Williamson, 1992). This test required drawings, written explanations, and choosing multiple choice explanations of chemical phenomena. Noting the need for specially designed tools for assessment of visualization skills, we designed three types of multimedia examination questions: explanations of computer displayed visualizations, selection of a visualization (nanoscale animation, video of experiment, dynamic graph of macroscopic property) that shows a specific feature, and matching of a target visualization with one in a different representational form (Russell & Kozma, 1996). Bowen (1998) argued that since chemists use multiple representations (macroscopic, particulate, and symbolic) to solve problems, chemistry students need to develop problem solving skills across all three levels and special types of test items are required to assess these skills. Bowen suggested examples of test items involving explanations of videos of chemical phenomena, animations of atoms and molecules during chemical or physical changes, and combinations of these with traditional test questions that feature symbolic representations. The following discussions of tools for assessing learning from use of multimedia chemical visualization software focuses on the expert-like visualization skills we believe should be developed in undergraduate chemistry curricula as discussed in the earlier chapter (Kozma & Russell, this volume).

3.1 Multimedia Test Items to Assess Conceptual Understanding and Visualization Skills

We have developed a variety of multimedia test items to use for the assessment of conceptual understanding and visualization skills (Russell & Kozma, 1996; Russell & Geno, 2000). Our earlier studies (Kozma & Russell, 1997) showed that test items requiring students to supply answers rather than choosing between possible answers are more likely to cause them to look beyond the surface features of the visualizations and produce responses based upon their views of the underlying chemistry. In the following paragraphs, we provide a number of examples of multimedia test items. All these examples require short free format responses. As we discuss these sample text items, we classify each question as a process question if it focuses on a visualization skill routinely used by chemists or as a conceptual question if its focus is on a fundamental chemical concept. Conceptual understanding may aid in answering process questions and hopefully the various visualizations will trigger the identification and application of an appropriate concept for the conceptual questions. Conceptual questions address learning from the cognitive theory perspective while process questions address learning from both cognitive and situative theory perspectives.

Figure 9 shows a series of screens taken from an animation depicting the equilibrium between liquid water and water vapor in a closed container. The animation begins with all molecules moving about in the lower layer representing liquid water. Soon molecules begin escaping into the vapor phase and returning to the liquid phase with on average three molecules shown at all times in the vapor phase. As this animation is displayed with a data projector on a large screen in front of the class the students have a printed test that shows one screen still to represent the animation. Next to this still shot is a model of water labeled H_2O.

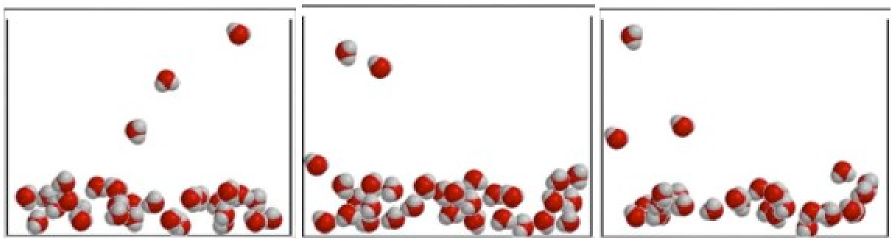


Figure -9. Three frames from animation of equilibrium between liquid water and water vapor.

Test items associated with this animation are:

1. Write an equation to represent the phenomena illustrated in the animation.
2. Describe how each species in the equation you wrote in part 1 is represented in the animation.
3. Does this animation show a dynamic equilibrium?

4. What could you do to this system to get more species into the upper part of the container?

These first two questions are designed to assess the student's ability to interpret a nanoscale animation and to transform this symbolic representation into the symbolic chemical equation. Although these questions require conceptual understanding of liquids and gases, they are classified as process questions with their focus on interpretation of nanoscale models and construction of an appropriate chemical equation. Students' responses might indicate their understanding of the concept of a dynamic equilibrium. The second pair of questions is strictly conceptual testing student's understanding of dynamic equilibrium and of vapor pressure and/or heats of vaporization.

The next example shows a test item that uses both a video of an experiment and a chemical equation for the reaction and asks responses in written language. The experiment starts with 100 mL of vinegar in four 250 mL volumetric flasks with attached balloons containing various masses of baking soda. The balloons are shaken to drop the baking soda into the vinegar. The masses of baking soda were chosen such that vinegar is the limiting reactant in two and baking soda the limiting reactant in the other two.

Figure -10. Specified masses of $NaHCO_3$(s) are added to 100 mL samples of vinegar resulting in the reaction, $NaHCO_3$(s) + CH_3COOH(aq) _ $NaCH_3COO$(aq) + H_2O + CO_2(g).

The printed test item shows the final frame of the video shown on the right in Figure 10. Next to this picture is printed the caption to Figure 10 giving the chemical equation. Three questions that have been used with this video are:

1. Why do the balloons inflate?

2. Does the HCO_3^- ion act as an acid or a base?
3. Why do the red and orange balloons inflate to the same volume but the yellow and blue balloons inflate to smaller volumes?

Although this experiment shows the limiting reactant concept, questions 1 and 3 can be answered by interpretation of the experiment as one forming a gas with the amount produced dependent upon the quantities of reactants available. The chemical equation confirms the formation of a gas and identifies it as CO_2. A complete answer to question 3 based only on observation of the video will state the limiting reactant concept whether or not students use the term limiting reactant. These two questions are classified as process questions. Question 2 requires understanding of Bronsted-Lowry acids and bases and is classified as conceptual.

Figure 11 shows three frames from animations showing the partial dissolving of $Cu(IO_3)_2(s)$ and total dissolving of $CuSO_4(s)$. For the partially soluble salt most of the ions remain in the solid phase shown as the regular array at the bottom of the frame. Ions in the solid continuously exchange with ions in the solution to maintain the constant saturated concentrations. The soluble salt results in all the ions moving throughout the solution.

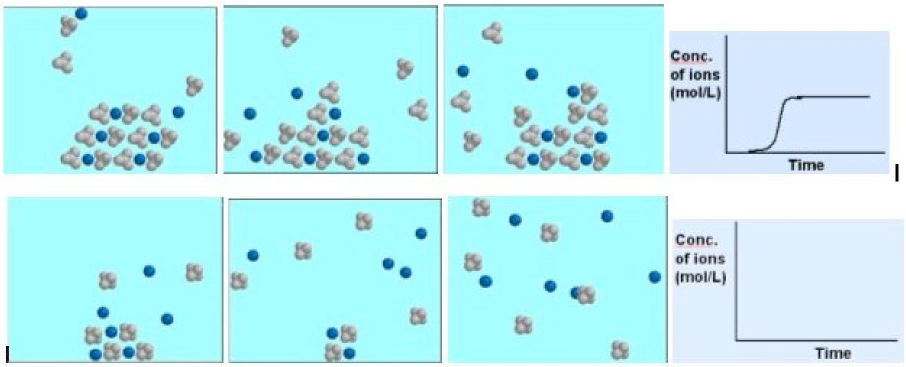


Figure -11. Three sequential screen shots from animations showing partial dissolving of $Cu(IO_3)_2(s)$ forming a saturated solution in upper sequence and total dissolving of $CuSO_4(s)$ to give an unsaturated solution in lower sequence. Upper graph shows change in concentration of Cu^{2+} with time. Graphs are used in question 3 below.

These two animations are played simultaneously before students answer the following three questions:

1. Explain the difference in the addition of $Cu(IO_3)_2(s)$ and of $CuSO_4(s)$ to water depicted in these animations.
2. Do either (or neither) of these examples show a dynamic equilibrium?

3. The change in concentration of $Cu^{2+}(aq)$ for the addition of $Cu(IO_3)_2$ to water is shown on the graph (Figure 11 upper). Add to this graph a curve representing the corresponding change in concentration of $IO_3^-(aq)$. On the other graph (Figure 11 lower) draw two curves representing the changes in the concentrations of $Cu^{2+}(aq)$ and $SO_4^{2-}(aq)$ for the addition of $CuSO_4(s)$ to water.

Questions 1 and 3 can be answered by observing the two animations without understanding the underlying concepts of identities (specific ions and solubility) and are thus classified as process questions. These questions can be answered based solely on the ability to interpret a nanoscale animation and to convert this representation to a graphical representation. Question 2 requires a conceptual understanding of dynamic equilibrium and is classified as conceptual.

Student responses to visualization items can be interpreted as assessing *both* student's conceptual knowledge and their ability to interpret and transform various types of visualizations. The following items show examples of responses of two students, whom we identify by the pseudonyms Sue and Joe, to three parts of the questions on water vapor equilibrium and HgO decomposition illustrated in Figures 9 and 4 respectively.

1a. Write an equation corresponding to the phenomena shown by this animation.

Sue: $H_2O(l) \rightleftharpoons H_2O(g)$
Joe: $H_2O(s)$ _ $H_2O(g)$

Sue correctly interprets the animation as showing liquid and gaseous water and is able to express this in terms of a chemical equation showing the symbol for equilibrium. Joe interprets the water molecules moving throughout the lower layer as a solid and shows an equation for a one way reaction. Sue has the expert's ability to interpret the animation and write a chemical equation. Joe wrote an equation that corresponded to his interpretation of the animation. The interpretation of the animation and its expression as a chemical equation is classified as a visualization (process) skill.

1b. How are all species in your equation represented in the animation?

Sue: Liquid H_2O is at the bottom with the molecules close together and moving around. H_2O gas is at the top with the molecules far apart and moving very quick.

Joe: Yes, $H_2O(s)$ and $H_2O(g)$

Sue is able to express her interpretation of the animation in written language. Joe does not answer the question merely noting without identification the presence of $H_2O(s)$ and $H_2O(g)$. This is a chemical process question addressing transformation from the symbolic animation to an alternate symbolic system – language.

1c. Explain how this animation illustrates a dynamic equilibrium.

Sue: Some of the liquid molecules went into the gas form and some of the gas molecules went into the liquid form. The same number that went into the gas is the same number that went into liquid.

Joe: The substance reactant _ product is constantly going at equal rates and the concentrations of reactant and products stay same.

This is a purely conceptual question requiring prior knowledge which both students have. By viewing their pretests we can determine if they had this knowledge before taking this course or acquired it during the course.

Question 9 below refers to the SMV:Chem experiment for the determination of the empirical formula of Hg_xO_y. One screen shot from this experiment is shown in Figure 4.

9a. Write a chemical equation for the reaction.

Sue: Hg_xO_y _ $xHg(l) + (y/2)O_2(g)$

Joe: HgO_2 _ $Hg + O_2$

Sue used the formulas on the graph to write a balanced equation showing the physical states of the two products. Joe wrote a balanced equation for a nonexistent oxide of mercury. These responses are to the process aspect of writing chemical equations from information supplied in a different representational form.

9b. How is the law of conservation of mass illustrated?

Sue: Each bar in the graph, when added together, still equals the same amount as the starting amount.

Joe: You end up with what you started with. Nothing is lost.

Sue correctly interprets the right hand graph showing constant total mass and expresses this correctly in words. Joe states, “nothing is lost” when the animation clearly shows oxygen is lost. If Joe is referring to the right-hand graph, then “nothing is lost” could mean no mass is lost. This question requires knowledge of the concept of conservation of mass and the skill to interpret graphs and/or animations. Both students focused on the graph. Although it is possible that students could using the right-hand graph figure out what conservation of mass means without prior knowledge, we classified this question as a conceptual question.

9c. If the experiment were stopped at the position indicated in the graph and animation with the mass determined by weighing the tube and subtracting the mass of the empty tube, what mass would be determined? (Express your answer to the nearest 0.1 g.)

Sue: The mass determined would be of Hg_xO_y and Hg.
$1.0\ g + 1.4\ g = 2.4\ g$
Joe: 1.4 g because everything in the tube is Hg_xOy.

Sue drew horizontal lines on the graph to estimate the masses of Hg_xO_y and Hg. Joe ignored the fact that the animation showed all the Hg formed remained in the tube. This question is a process question testing the ability to interpret the graph and the animation.

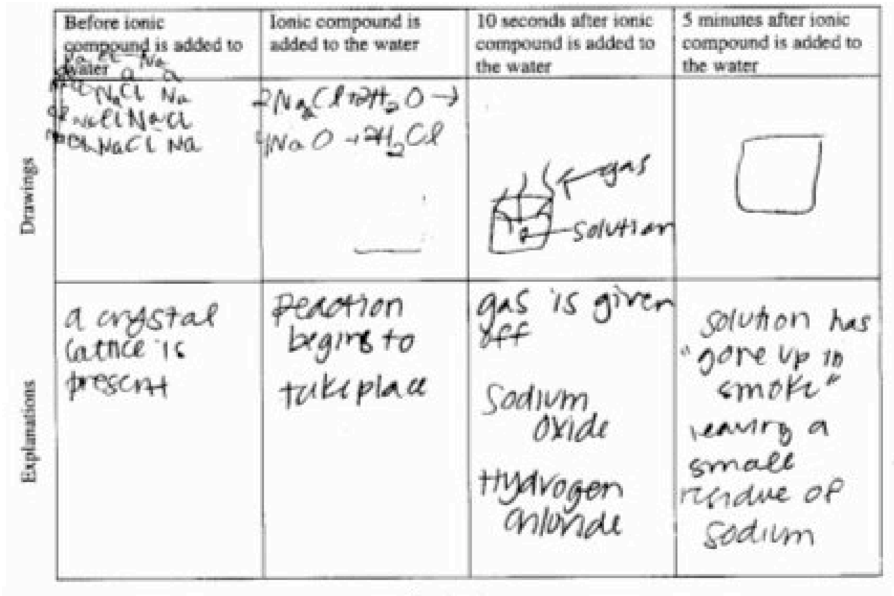
These questions illustrate how tests of this type can both assess components of students’ conceptual knowledge and their abilities to perform the processes associated with doing chemistry. Some questions about chemical processes can be formulated using still images like the three frames for the liquid water and gaseous water equilibrium question, as shown in the prior section of this chapter, but the questions are much clearer if they are shown as an animation movie. All of the questions on this test involve some parts that require a transformation from one form of representation to another – a processing skill chemists must develop. Ten multiple-part questions used on the visualization tests discussed below are included on the sample test shown on the accompanying CD-ROM. The test section on the CD-ROM contains a MS-Word document that serves as the test booklet and a MS PowerPoint presentation that has been compressed with Impatica. In the compressed form all visualization movies will play as soon as the slide containing them is opened. When used in the PowerPoint form for an in-class test, the instructor can start each movie and replay them as needed.

3.2 Assessment of Representational Competence after Use of *ChemSense*

In a study involving the use of *ChemSense* in a high school chemistry course (Schank & Kozma, 2002), we found a significant increase in representational skills and a movement from using representation as depiction to using representations to describe, explain, and predict what was happening at the nanoscopic chemical level.

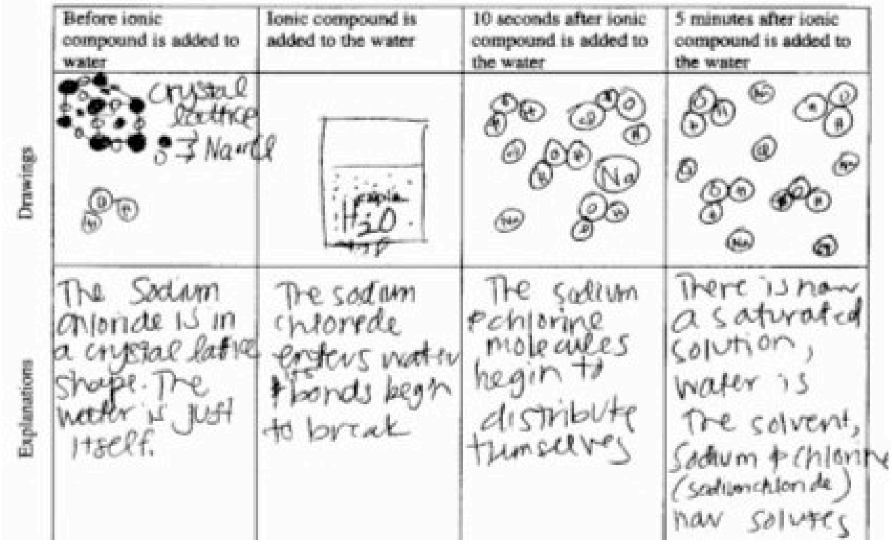
To provide a more detailed picture of how representational competence can be assessed, we present a test item example and work though the scoring of student's representational competence. [See earlier chapter (Kozma & Russell, this volume) for a discussion of "representational competence".] The item for this example is a four-step "storyboard" question asking students to draw and explain at the nanoscopic level how NaCl dissolves in water over time. This item allows students the opportunity to show their understanding of a solubility-related *process* and represent it accordingly. Students were scored on both their chemical understanding and their representational competence. Here we compare pretest and posttest responses for a given student only for representational competence. In the earlier chapter we defined representational competence and provided a five level scale for representational competence: Level 1 – representation as depiction, Level 2 – early symbolic skills, Level 3 – syntactic use of formal representations, Level 4 – semantic, social use of formal representations, and Level 5 – reflective, rhetorical use of representations.

Figure 12 shows a sample pretest response for our example test item. At pretest, the student completed all frames of the storyboard. However, instead of creating nanoscopic-level representations, the student provided a macroscopic-level drawing of the solution and a representation of the ionic lattice using the symbols "Na" and "Cl" to represent nodes in the lattice. This is evidence that the student is operating at a "surface level" representational competence—the discussion centers only on observable, macroscopic level features. The student uses representations as depictions of what they might see at the lab bench, providing only an "isomorphic, iconic depiction of the phenomenon at a point in time." This student's response at pretest received a "level 1" score.



	Before ionic compound is added to water	Ionic compound is added to the water	10 seconds after ionic compound is added to the water	5 minutes after ionic compound is added to the water
Drawings	NaCl Na NaCl NaCl NaCl Na	$2NaCl + 2H_2O \rightarrow$ $4NaO + 2H_2Cl$	gas solution	
Explanations	a crystal lattice is present	Reaction begins to take place	gas is given off Sodium oxide Hydrogen chloride	solution has "gone up in smoke" leaving a small residue of sodium

Pretest



	Before ionic compound is added to water	Ionic compound is added to the water	10 seconds after ionic compound is added to the water	5 minutes after ionic compound is added to the water
Drawings	crystal lattice Na Cl	H_2O	Na	
Explanations	The Sodium chloride is in a crystal lattice shape. The water is just itself.	The sodium chloride enters water & bonds begin to break	The sodium & chlorine molecules begin to distribute themselves	There is now a saturated solution, water is the solvent, Sodium & chlorine (sodiumchloride) now solutes

Figure -12. Sample pretest (upper) and posttest (lower) for student using ChemSense.

At posttest this student demonstrated a richer, more complex representation of the underlying process. Here the student correctly used space filling molecules to represent the underlying, non-observable entities and processes, and provided an accurate description of the dissolving process except for showing atoms rather than ions as the solutes. The student shows a semantic and social use of formal representations, using these representations to explain the physical phenomena rather than simply depicting what may be seen and the response was scored at a "level 4."

3.3 Studies of Efficacy of SMV:Chem for Enhancing Visualization Skills

We used multimedia visualization test items as discussed above as components of assessment instruments for studies of the efficacy of *SMV:Chem* in the classroom and for out-of-class assignments. Three recent studies (Russell, 2004) are summarized. The first two studies conducted during the 2001-2002 academic year involved six sections of a first semester general chemistry course taught by five different very experienced instructors. We distinguished the fall 2001 and winter/spring 2002 studies for two reasons: fall and winter semester students typically are drawn from different groups as confirmed by their pretest scores in these studies and we used extra questions on the winter/spring pre- and posttests. One section each term taught by instructors A and B used no *SMV:Chem* components and served as control sections. Instructor C taught one section in fall 2001 using eight *SMV:Chem* homework assignments with occasional use of videos and animations from *SMV:Chem* in lectures. Instructor D taught one section in the fall, winter, and spring semesters using four SMV:Chem homework assignments and made extensive use of software visualizations during lectures. A sample of one of the SMV:Chem homework assignments used in these studies is included on the CD-ROM as well as examples of three homework assignments in the new Version 3.0 web-based format. Additional homework assignments may be viewed at http://www2.oakland.edu/users/russell.

Prior to discussing the results of these studies, we report on a subset of the data from the Winter 2002 study that shows one measure for comparing the overall performance in first semester general chemistry of students in the control and experimental sections. This comparison also shows the correlation between the visualization skills measured on our test and performance on a standardized chemistry examination. The American Chemical Society's Examination Institute has developed conceptual questions that contain limited assessments of visualization skills within the limitations of a printed multiple-choice format exam. We have compared student performance on the 2000 ACS First Semester General Chemistry exam with both conceptual and quantitative questions with performance on tests we have constructed to assess visualization skills (Russell, 2002; Russell, 2004).

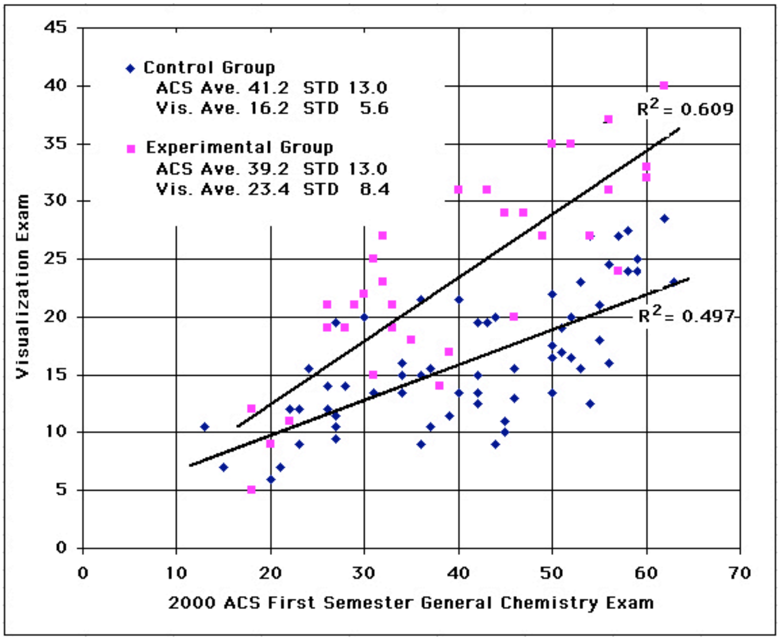


Figure -13. Correlation of scores on visualization test and ACS 2000 First Semester General Chemistry Test. Experimental group used four SMV:Chem homework assignments and control group used none.

Figure 13 shows correlations between scores on the ACS exam (70 points) and our ten multiple-part question visualization test (43 points) for two sections (experimental, n = 34; control, n = 62) of first semester general chemistry taught by two instructors in Winter 2002. As shown by t-tests (two-tailed, two samples with unequal variance), the differences in scores on the visualization test were significant (p = 0.0002) but insignificant on the ACS exam (p = 0.45). The data in Figure 12 show not only is the average score on the visualization test higher for the experimental group but visualization test scores are higher across the range of ACS exam scores. The data show that students with ACS scores less than 25 had similar performance levels on the visualization test. The increased slope of the linear least square line for the experiment group compared to the control group showed use of the *SMV:Chem* assignments was more effective for higher ability (as measured by the ACS exam) students. The R^2 values of the two least squares regression lines show a slight increase in the correlation between visualization test and ACS exam scores for the experimental group compared to the control group.

For all six sections in the Fall 2001 and Winter/Spring 2002 studies a pre- and posttest methodology was used with the pretest given during the first week recitation section. The posttest for the control groups was given during the last week recitation section and for the experimental groups was part of the final exam. To encourage students to provide their best efforts on the pretest and the control group posttests extra credit points toward their total course grade were awarded to students who made serious efforts to answer every question. A copy of the 2002-2003 test is included in the Russell-Kozma section of the CD-ROM. For all sections in the 2001-2002 study the first six questions were used on the pre- and posttests. For the winter and spring 2002 sections, questions seven and eight were added. The fall tests were scored based upon a total of 25 points with 10 points for process questions and 15 points for conceptual questions as discussed above. The winter/spring test had 30 points with 13 process and 17 conceptual. Results for the 2001-2002 study are shown in Table 1.

Table -1. 2001-2002 sections of first semester general chemistry. Average differences in posttest and pretest scores for all questions, for process questions, and for conceptual questions with respective (standard deviations). The last three columns show t test p values for comparing each experiment group with its control group.

Sect.	Inst.	No	Post-Pre (25 pts) Total	Post-Pre (10 pts) Process	Post-Pre (15 pts) Concept	T test p Total	T test p Process	T test p Concept
F01 Contr.	A	58	5.66 (3.14)	2.58 (1.83)	2.98 (2.160			
F01 Exp.8	C	40	8.21 (3.87)	4.24 (2.30)	3.98 (2.68)	$6\mathrm{x}10^{-4}$	$3\mathrm{x}10^{-4}$	0.06
F02 Exp.4	D	33	8.82 (3.33)	3.88 (2.04)	4.94 (2.27)	$2\mathrm{x}10^{-5}$	0.003	$2\mathrm{x}10^{-4}$
			Post-Pre (30 pts) Total	Post-Pre (13 pts) Process	Post-Pre (17 pts) Concept			
W02 Contr.	B	63	3.35 (3.33)	2.52 (1.96)	1.03 (2.42)			
W02 Exp.4	D	30	6.95 (4.58)	2.63 (2.05)	4.32 (3.32)	$7\mathrm{x}10^{-4}$	0.79	$2\mathrm{x}10^{-5}$
Sp02 Exp.4	D	17	7.94 (5.72)	4.18 (2.78)	3.76 (3.91)	0.007	0.03	0.01

The differences between the average increases in pretest to posttest overall scores were statistically significant at the $p < 0.01$ level for all experimental groups compared with their control groups. The most interesting conclusion from the t test p values for the separated process and conceptual questions is that except for the eight homework fall 2001 section the pretest posttest gains between experimental and control groups were more significant for the conceptual questions. However, there were some confounding factors in this study. For example, students in the group who received eight homework assignments had used all of the visualizations that appeared on the posttest while answering different questions in the homework assignment than used on the visualization test.

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In order to eliminate a number of these confounding issues another study was performed in 2002-2003. Since the earlier study showed fairly consistent pretest scores for all sections of first semester general chemistry, the pretest was eliminated. This meant that no student had seen the posttest questions before the posttest. Both instructors for the experimental sections agreed to use five homework assignments chosen to minimize exposure to experiments covered on the posttest. Instructor C used different parts of *SMV:Chem* experiments covered on 22% of the posttest questions while instructor D used a different part of one experiment covered on 4% of the posttest questions. Questions seven and eight on the visualization test shown on the CD-ROM used in the 2001-2002 studies and covered in the lab and homework assignments were replaced by questions nine and ten not covered in the homework. Table 2 summaries the results of this study.

All experimental posttest scores for overall questions, process questions, and conceptual questions are significantly higher than their control sections at the $p < 0.0001$ level. The posttest score for the winter 2003 control group and fall 2002 experimental groups are essentially the same for all questions, process questions, and conceptual questions. It appears the gains in visualization skills acquired through use of *SMV:Chem* homework assignments during the first semester of general chemistry are matched by students who did not use the software after two semesters of general chemistry. Students who used the software during the second semester showed additional gains for both process and conceptual questions.

Table -2. Average posttest scores for all questions and for process and conceptual questions for CHM 157 and 158, 1st and 2nd semesters of general chemistry, with (standard deviations). t test p values compare row and column sections for total questions.

Sect.	Inst.	No	Posttest (38 pts) Total	Posttest (19 pts) Process	Posttest (19 pts) Concept	T test p F02 Contr.	T test p F02 Exp.	T test p W03 Contr
F02 Contr. C157	B	50	13.12 (3.92)	5.68 (2.07)	7.44 (2.66)			
F02 Exp.5 C157	C	34	19.16 (6.61)	9.27 (3.76)	9.90 (3.52)	$2x10^{-5}$		
W03 Contr C158	E	32	18.81 (6.49)	9.30 (3.97)	9.42 (3.01)	$5x10^{-5}$	0.83	
W03 Exp. 5 C158	D	29	26.84 (5.59)	13.09 (3.29)	13.72 (3.14)	$4x10^{-15}$	$5x10^{-6}$	$3x10^{-6}$

The scoring for the eight questions used in the 2002-2003 study (questions 1-6, 9,10 of visualization exam included on the CD-ROM) were equally divided between questions judged as process and conceptual as discussed above. Table 3 shows that for all sections students showed nearly identical performance on process questions and conceptual questions. Thus although *SMV:Chem*'s design conforms to Mayer's principles for multimedia learning tools to enhance conceptual understanding it's use also contributes to the acquisition of skills used by chemists as they interact in work environments consistent with situative theory.

4. FUTURE DIRECTIONS OF VISUALIZATIONS IN CHEMICAL EDUCATION

4.1 Recommendations for the Development of Visualization Software

Over the last 10 years, there has been a significant amount of development of visualization software in chemistry. Molecular modeling software packages, such as *Spartan, Hyperchem, Gaussian+GaussView, etc.*, are being successfully used in undergraduate college and even high school chemistry courses for their visual and numerical results without requiring understanding of their theoretical basis. As reported above, several large-scale visualization packages have been specifically design for chemistry education, often with the support of the U.S. National Science Foundation. Many of these packages involve simulations and animations of molecular systems and the use of multiple representations. Results from initial studies of these packages warrant continued support for their development and scaling up.

Modeling tools usually display the structure of a single molecule. These tools are important in helping students understand the structure and properties such as dipole moments and energy states of molecules. Simulations help students understand difficult concepts related to the dynamics, rate, concentration, etc. of chemical systems that involve relatively large numbers of molecules and reactions. We feel there is an important place for simulations of single reactions. Simulations of reactions based on the electronic structure methods showing transformations of molecular (frontier) orbitals, electrostatic potentials, electron densities, etc., during reactions will aid the visualization of single reactions.

Many of the Chime-format models now available are built using data for atomic coordinates available from web-based databases: Inorganic Crystal Structure Database, http://fiz-informationsdienste.de/en/DB/icsd/; Cambridge Structural Database for small molecules, http://www.ccdc.cam.ac.uk/products/csd; Protein Data Bank, http://rcsb.org/pdg/; Nucleic Acid Database, http://ndbserver.rutgers.edu; and Crystmet database for metals and alloys, http://www.tothcanada.com.

4.2 Recommendations for Visualization-Based Instructional Activities

Our review of the research and development literature warrants the use of visualization technologies in chemistry instruction. These findings are strongest when the instructional goal is to teach concepts and principles. We identified instances in which lectures were supplemented by animations to successfully teach concepts related to equilibrium, reaction chemistry, electrochemistry, and miscibility. (See also Kozma & Russell, this volume.) We found studies in which molecular models supported students' understanding of structure and bonding. Several significant development projects, such as *SMV:Chem, Connected Chemistry,* and *Molecular Workbench*, provide instructors and instructional designers with new technological resources to bring multimedia into the chemistry classroom. However, the current state of research on chemical visualization does not allow us to say much beyond this. There are no carefully designed experiments that tell us when it is best to use animations versus still pictures or whether dynamic molecular models are better than physical ball-and-stick models. Nor can we say with much precision how these various media can be used together and when it is best to do so. For the time being, all of these practical issues are left up to the judgment of instructors and instructional designers.

The current research allows us to say even less, if the goal is to teach chemistry as a process of investigation. Situative theory would argue for the use of various representations in the context of laboratory investigations, using them to ask questions, plan experiments, carry out procedures, analyze data, and present findings. New software systems, such as *ChemSense* and *ChemDiscovery*, provide instructors with powerful tools to support students' investigations. Initial studies with these environments seem to suggest that they foster the kinds of investigative activities that are encouraged by the theory. But there is little systematic research so far that helps guide instructors and instructional designers on how to effectively integrate these tools into classroom and laboratory activities.

4.3 Recommendations for Testing Activities

Almost all of the studies that we examined used specially designed tests which measured students' understanding in new ways and measured new goals for chemistry learning, such as increasing students' abilities to use appropriately diverse forms of representations in problem solving as are used by experts. Indeed, in the experimental studies we reviewed, visualizations had the greatest effect on test items of this sort. These findings argue for the integration of still pictures, animations, models, and other visualizations into the tests and examinations of chemistry courses. There are now a variety of multimedia tools that make it easy for chemistry instructors to include these kinds of items in their regular student assessment activities.

ACKNOWLEDGEMENTS

Robert Kozma's participation in this chapter was made possible by the National Science Foundation under Grant No. 0125726. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

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