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Students Becoming Chemists: Developing Representational Competence

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Over the past decade or so, there has been a significant effort to change the curricular goals of science education in the U.S. At the postsecondary level, science agencies (American Association for the Advancement of Science, 2001; National Research Council, 1996b; National Science Foundation, 1996) have promoted literacy in science, mathematics, and technology by direct experience with the methods and processes of inquiry. At the primary and secondary levels, national science standards emphasize the learning of science as both as a process of investigation, as well as a body of significant concepts (American Association for the Advancement of Science, 1993). For example, the National Research Council (1996a) states that a new vision of science standards "requires that students combine processes and scientific knowledge as they use scientific reasoning and critical thinking to develop their understanding of science. . . Science as inquiry is basic to science education and a controlling principle in the ultimate organization and selection of students' activities" (p. 103).

In this chapter, we examine new visualization technologies in chemistry and consider the implications that these technologies and the above stated goals have for helping students become chemists. Clearly, very few high school and college students actually go on to major in a science and even fewer go on to major in chemistry. Nonetheless, a strong case can be made for using the investigative practices of scientists as the orienting themes for the science curriculum (O'Neill & Polman, 2004). Traditionally, the primary focus of the chemistry curriculum has been students' acquisition of significant chemical concepts, such as bonding, structure, reactivity, equilibrium, oxidation, acidity, and so on. An overemphasis on concepts has lead to a curriculum in the U.S. that is sometimes characterized as a "mile wide and an inch deep" (Vogel, 1996, p 335). The new goals expressed above do not replace the acquisition of concepts, although they may compete for limited time in the curriculum. Rather, they shift the emphasis to the acquisition and use of concepts within the context of scientific investigation in which students pose research questions, design investigations and plan experiments, construct apparatus and carry out procedures, analyze data and draw conclusions, and present findings (Krajcik, et al., 1998). Within this context, students have a deeper understanding of (perhaps fewer) concepts because they are the focus of intensive investigation. But perhaps more important, with these goals students also come to understand the basis for scientific claims and theories related to these concepts (O'Neill & Polman, 2004).

In the following sections, we look at the role of visualizations for both kinds of goals for chemical education: those related to the acquisition of significant concepts and those related to scientific investigation. However, our emphasis is on the use of visualizations to support students' investigative practices and to develop a set of skills that we call "representational competence". Specifically the goals of this chapter are:

- examine the representational skills and practices that chemists use while conducting scientific investigations.
- compare these representational skills and practices to those of chemistry students.
- review related theories of learning.
- consider the implications of these research findings and theory for the new goals of chemical education and the development of students' representational competence.

- review research related to several kinds of visualization technologies that can promote learning in chemistry.
- propose recommendations for changes in the chemistry curriculum and for future research in chemical education, based on these theories and research results.

To achieve our goals, the chapter is divided into six major sections: chemists' uses of visualizations; students' uses of visualizations; theories of learning; new goals for chemical education; research on visualizations in chemical education, including molecular modeling, simulations, and animations; and implications for the chemistry curriculum and future research on visualization in chemical education. In the subsequent, companion chapter (Russell & Kozma) we describe a number of specific visualization software environments and assessment systems.

Chemists' Uses of Visualizations

Eminent chemist and former President of the National Science Board, Richard Zare (2002, p. 1290) characterizes chemists as ". . . highly visual people who want to 'see' chemistry and to picture molecules and how chemical transformations happen." There are two types of representations that chemists use to understand chemical phenomena, those that are internal, mental representations and those that are external symbolic expressions. All chemists have developed the ability to "see" chemistry in their minds in terms of images of molecules and their transformations. In this chapter we refer to such internal representations as concepts, principles, or "mental models" that encompass the state of chemical understanding of the individual. Chemists also construct, transform, and use a range of external representations—symbolic expressions, such as drawings, equations, and graphs. In conversations between chemists they spontaneously draw equations and structural diagrams to visually depict components of their mental models and the composition and structure of the compounds that are the object of their work. Indeed, Nobel chemist Roald Hoffmann contends that, "In an important sense, chemistry is the skillful study of symbolic transformations applied to graphic objects" (Hoffmann & Laszlo, 1991, p.11). In this chapter, we refer to such symbolic expressions as "visualizations" or merely "representations" (Kozma, Chin, Russell, and Marx, 2000). (Others refer to them as "inscriptions"; see Roth & McGinn, 1998.) Thus visualizations are perceptible, symbolic images and objects in the physical world that are used to represent aspects of chemical phenomena, much of which can not be seen. In this sense the representations that Zare "sees" within his mind are mental models while the figures he draws on paper or constructs on a computer screen are visualizations.

An Historical Analysis

The role of representations and visualization technologies are central to the development of chemical understanding—not just the understanding of students as they struggle to learn about aperceptual chemical entities and processes but central to the understanding of chemists and, indeed, to the development of the field. There has always been a strong relationship between chemists' understanding of chemical phenomena and the external representations that they use to represent them. In a short historical review of representation in chemistry (Kozma, Chin, Russell, & Marx, 2000), we found that in the development of the discipline, new representations and tools have corresponded to new approaches to the study of chemical substances and new ways of thinking about the aperceptual chemical entities and processes that underlie and account for the material quantities of these physical substances. Within a community of shared goals, knowledge, activities, and discourse, chemists came to use these new representations and tools and they, in turn, shaped the way chemists thought about and conducted their work.

This process is most dramatically illustrated in the late 18th century when chemistry became a modern science. What distinguished pre- from modern chemistry was the transformation from the practice of conducting qualitative experiments (such as noting that a red mineral changed to a silver liquid upon heating) to quantitative experiments (such as noting that 100 g of the red solid produced 86.2 g of the silver liquid). This quantitative approach facilitated a change it the way chemistry was represented, a change in the most fundamental way that any field is represented—its language. Prior to the work of 18th century chemist Anton Lavoisier and his contemporaries, chemicals were named based upon their physical properties. The red solid, HgS, was called vermilion and the silver liquid, Hg, quicksilver. By the late 18th century Lavoisier and others began to establish analytic techniques needed to find the underlying composition of substances as the focus of chemistry. At the same time, Lavoisier, Guyton de Morveau and colleagues developed a nomenclature system based upon elemental composition rather than physical properties (Anderson, 1984). For Lavoisier the connection between the development of the language and new activities within the discipline was explicit. Specifically, the naming of a substance required its experimental decomposition so that the component elements could be identified. The evolution of the chemical formula allowed chemists to display how molecules decomposed and combined and these symbolic expressions corresponded to the experimental procedures used in the laboratory to decompose and combine physical substances. Thus the language and symbol system were structured such that operating on symbols would be analogous to operating on substances. By embedding in chemical nomenclature and symbol systems a shift in focus from physical surface features to aperceptual elemental composition, Lavoisier created a new way of thinking about chemistry, a new set of practices, and a new chemical community. Lavoisier stated that:

> A well formed language, a language in which one will have captured the successive and natural order of ideas, will bring about a necessary and even prompt revolution in the manner of teaching. It will not allow those who profess chemistry to diverge from the march of nature. They will either reject the nomenclature, or else to follow irresistibly the route that it will have marked out. (as cited in Anderson, 1984, p. 176).

Developments in chemistry have continued to be shaped by developments in the way chemical phenomena are represented or visualized. In the 20th century chemical synthesis—the design and formation of molecules—became a major emphasis of the field. In parallel with this new activity was the development of structural formulas or diagrams. Structural formulae show both the composition and the bonding pattern of atoms in molecules and such visualizations aid the analysis of sites within a compound that will react to form new molecules.

Between the 1930s and mid-1960s, chemists developed physical 3-D structural models composed of elemental components (sometimes balls) and (sometimes) sticks representing bonds between elements (Francoeur, 1997, 2002). These structures made the dimensional arrangement of elements more explicit and allowed for rotation and inspection of the molecule. With the advent of sophisticated computers and molecular modeling software beginning in the 1960s, it was very easy to construct ball and stick, space filling, and electron density models for even very large molecules. Such interactive molecular graphics have come to replace physical models. The advantage of the computer modeling programs is that they support additional analyses, such as measuring bond lengths and angles. At each stage in the development of more refined and meaningful models the new representations afforded new chemical practices and new ways of thinking about chemistry, such as considerations of chirality, steric factors, and electrophilic and nucleophilic species. The outputs of new tools (chromatographs, infrared spectra, NMR spectra, mass spectra) also provided graphical visualizations of physical properties of the aperceptual molecules that supported the synthesis of new compounds.

An Ethnographic Study of Chemists

These historical examples illustrate that the design and use of visualization systems is a key cultural activity that affects the composition of a community, the activities of its members, and the understanding its members share about its domain of knowledge. In our ethnographic study of chemists we described how this finding is realized in everyday chemical practice (Kozma, Chin, Russell, & Marx, 2000). In this study, we investigated the interplay between various forms of visualization and the practices and discourse of chemists at an academic and a pharmaceutical laboratory, both focusing on the synthesis of new compounds.

In the academic lab we observed two graduate students, a postdoctoral fellow, and a faculty mentor as they worked and in the pharmaceutical lab six chemists including one project director were observed working at the bench and participating in group problem-solving meetings. For all these synthetic chemists, in every conversation, and written on laboratory hood doors and on white boards in conference and coffee rooms, chemical equations using structural formulae were omnipresent. The next most common forms of visualizations used by chemists in both settings were nuclear magnetic resonance (NMR) and mass spectra. These visualizations served two important, interrelated roles in the practices of chemists: material and social. First, visualizations provided a material representation of otherwise aperceptible entities and processes, representations that could be perceived and manipulated. Second, visualizations served to support the social discourse of chemists as they worked to synthesize intended compounds.

There were several patterns in representational practices that we noticed in our observations. First, chemists used visualizations to express their research goals in terms of molecular structures of compounds. That is, chemists used structural diagrams to describe the composition and geometry of the compounds that they were trying to synthesize. Second, they used visualizations to reason about the chemical and physical processes needed to synthesize these compounds. They used diagrams and equations to think though the possible reaction mechanisms by which reagents would be transformed to desired products and the physical procedures in the laboratory that would support these transformations. Third, chemists used visualizations to verify the composition and structure of the synthesized compounds. They would analyze instrumental displays and printouts to determine if the products were the compounds that they were trying to synthesize. Fourth, they used visualizations in a rhetorical sense to convince the scientific community that the compound they synthesized was the one intended. In this regard, specific features of the printouts were used as warrants for claims that that the products were indeed structured as intended. Finally, chemists' use of various visualizations confirmed their membership in the scientific community. This is, by using various representations in these ways, graduate students and postdoctoral fellows developed the chemical skills and practices that integrated them into the community of chemists.

Students' Uses of Visualizations

The various ways that chemists visualize chemical entities and processes differ significantly from the ways chemistry students use representations. They differ both in their laboratory practices and in their ability to use and understand various forms of visualization.

An Ethnographic Study of Students

In an observational study of an organic chemistry course, we examined the laboratory practices of college students (Kozma, 2000b, 2003). Pairs of students were audio and video recorded as they interacted with each other while synthesizing a compound in the laboratory. We analyzed their actions and interactions during one laboratory session and found several patterns. First, in sharp contrast to academic and professional laboratory practice, we found infrequent use of visualizations by students during their wet lab experiments. As a consequence, the laboratory practices and discussion of chemistry students was focused on the physical aspects of their experiments—the laboratory equipment and the physical properties of reagents. The discussion among student lab partners was focused primarily on setting up equipment, trouble shooting procedural problems, and interacting with the physical properties of the reagents they were using (e.g., was their crystalline product washed enough or dry enough). Second and most important, students rarely discussed the molecular nature of the reactions that they were running on the lab bench. Unlike the discourse of chemists, we observed very little discussion among students about the molecular properties of the compounds they were synthesizing or the reaction mechanism that might be taking place during their experiments. The lack of representational use even shaped the discourse of the laboratory instructors. In these discussions between students and their instructors, the mention of molecular properties and processes was absent.

An Expert Novice Study of Visualization

These differences between chemists and chemistry students in laboratory practices correspond to significant differences in chemists' and students' understanding of various forms of chemical visualization. In an earlier study (Kozma & Russell, 1997), we examined what expert chemists and novice students understand when they see and use various chemical visualizations such as graphs, equations, and animations of molecular phenomena. We also wanted to know if subjects saw connections between different chemical visualizations corresponding to the same phenomena or if they understood something different for each type of visualization. The novice pool consisted of 11 first semester chemistry students from a Midwestern research university. The expert pool consisted of five doctoral students from this university, five chemists from a pharmaceutical company, and one community college instructor. All subjects were videotaped as they worked at a computer to complete two tasks.

Subjects were shown 14 dynamic and still images corresponding to several chemical reactions. The representations included videos of the experiments, animations of the molecular events, dynamic graphs of a physical property of the system, and chemical equation or formulae. Subjects were then given a card corresponding to each representation, with its dynamic image being represented by a single still frame. They were asked to sort these cards into logical subsets, give a name to each subset, and explain the meaning of the name. In this sorting experiment we observed that both experts and novices created chemically meaningful groups. However, novices formed their meaningful groups from a small number of cards often from the same media type (e.g., all graphs, all equations, etc.) while experts used larger groups composed of multiple media forms. Also the reasons for forming particular groups that experts gave were largely conceptual while novices' reasons often were based upon surface features.

In the second task subjects were shown various visualizations—chemical equations, videos of experiments, dynamic graphs of a physical property of some experiment, and animations of the molecular events of an experiment. They were asked to describe what they saw and then to transform the visualization into various other forms, as specified. (Digitized versions of these tasks are included on the CD with this book under the chemistry section, entitled sorting tasks and transformation tasks.) From this transformation experiment we found that experts were much better than novices at providing verbal descriptions, due to their deeper understanding of chemical principles and concepts. Experts were only slightly better than novices with transformations requiring a choice between answers (e.g., given an equation and matching it to one of several video segments), since surface features could be utilized to make a choice. However, they were much better than novices for transformations that required a constructed response such as drawing a graph or writing a chemical equation. They were particularly better in giving verbal descriptions as transformations.

Although this study used a variety of visualizations not used in prior expert-novice studies (Chi, Feltovich & Glaser, 1981; Glaser & Chi, 1988; Larkin, McDermott, Simon & Simon, 1980), its conclusions were consistent with these earlier studies. Experts in our study were able to use their deep conceptual knowledge and mental models of chemical phenomena to construct the meaning of these visualizations while novices based meaning on the surface features of the visualizations or the physical properties of the reactions. Experts as members of the chemical community not only have a more extensive knowledge base but they also were experienced in using diverse forms of visualization as they communicate with others.

Learning Theory and Visualizations in Chemical Education

Learning theory has also developed over the last several decades. The focus of learning theory in the 70's and 80's was on the mind of the individual learner—cognitive structures and processes. Beginning in the late 80's and early 90's, theorists focused on how learners interacted with the social and physical resources in their environment and how they integrated into communities of practice—what has come to be called "situative theory". Together these theories address the two types of goals for the chemistry curriculum. Cognitive theory has significant implications for how instruction could be designed to support the acquisition of concepts and problem solving procedures. Situative theory has implications for goals related to investigative practices and "becoming chemists". Both have implications for the use of representations and visualizations.

Learning Concepts

An important goal for chemical education is student acquisition of key concepts and principles, such as bonding, structure, reactivity, equilibrium, acidity, and so on. High school and even college students have significant difficulty understanding these concepts and principles (Gable, 1998; Krajcik, 1991; Nakhleh, 1992), in large part because they related to phenomena that are not available for direct inspection.

Mayer (2001, 2002, 2003) describes a cognitive theory of multimedia learning and proposes principles for the design of effective multimedia instruction to address the learning of concepts and principles. This important work was summarized for the chemical education community by Robinson (2004). Mayer uses three assumptions from cognitive psychology: dual channel, limited capacity, and active processing. The dual channel assumption states that the human brain has separate channels for processing auditory-verbal and visual-pictorial inputs (Baddeley, 1999; Paivio, 1986). The limited capacity assumption is that there is a relatively small limit to the part of the human brain called working memory that processes and manipulates inputs from the auditory-verbal and visual-pictorial channels (Baddeley, 1999; Johnstone, 1997). There are both limits to the amount of information that can be processes from each channel as well as a non-additive overall limit. Learning occurs when the student actively selects, organizes, and integrates information from auditory and/or visual inputs (Mayer, 2001). Mayer (2002) uses this theory and research findings from numerous studies to develop eight principles of multimedia learning that use both channels, address limited cognitive capacity, support students' active processing, and result in deeper learning—that is learning that results in understanding of difficult concepts and principles which can then be used to solve novel problems. These are:

1. *Multimedia Principle*. Deeper learning occurs when both words and pictures are used than from the use of words alone.
2. *Contiguity Principle*. Deeper learning results from presenting words and pictures simultaneously rather than successively.
3. *Coherence Principle*. Deeper learning occurs when extraneous words, sounds, or pictures are excluded rather than included.
4. *Modality Principle*. Deeper learning occurs when words are presented as narration rather than as on-screen text.
5. *Redundancy Principle*. Deeper learning occurs when words are presented as narration rather than as both narration and on-screen text.
6. *Interactivity Principle*. Deeper learning occurs when learners are allowed to control the presentation rate than when they are not.
7. *Signaling Principle*. Deeper learning occurs when key steps in the narration are signaled rather than nonsignaled.
8. *Personalization Principle*. Deeper learning occurs when words are presented in conversational style rather than formal style.

These eight principles have a direct bearing on how visualizations can be used in chemical education to support the learning of difficult chemistry concepts and principles. For example, the multimedia, contiguity, and modality principles encourage the simultaneous use of visualizations along with aural instruction to provide a synergistic learning effect by supporting the active processing of both visual and audio inputs in working memory. Multimedia software would be more effective if it used audio narration rather than printed text. The coherence and redundancy principles suggest that educators and instructional designers use the simplest possible visual and audio components to achieve the specific learning objective. Visualizations should reduce unnecessary details, rather than be as realistic as possible, in order to achieve a specific learning goal.

The cognitive theory and design principles described by Mayer (2001, 2002, 2003) and Robinson (2004) assume an educational model in which learning occurs as a result of the student's engagement with some instructional presentation, be it software or lecture. The focus is on learning difficult concepts and principles. When students interact with information that is represented in both pictures and words they are more likely to learn difficult concepts and principles, retain what they learn longer, and use what they learn to solve problems, than if the information is presented in words alone.

To illustrate the application of this theory to chemical education, a common organic chemistry convention is to represent unreactive portions of molecules as "wiggle lines", "picket fences”, or “R”; this convention would be useful for instructional purposes, as well, because it reduces extraneous information (*Coherence Principle*). Similarly, in a molecular animation, it is likely to be more effective to show the equilibrium reaction N_2O_4 _ $2NO_2$ by using single and double spheres of different colors rather than space filling models with unnecessary detail. The Personalization and Signaling Principles provide guidelines for writing and reading audio narration that accompanies visual representations of molecular processes. The Interactivity Principle supports numerous studies that favor active learning and software design with at least a minimum amount of user control over the rate of movement through the lesson. In a later section of this chapter and in the subsequent chapter (Russell & Kozma), these principles will be used in reviewing specific visualization studies and products.

Learning Investigative Practices

If the educational goal is to engage students in chemical practices of laboratory investigation then visualizations need to be used in a different way than that proposed by Mayer. Correspondingly, a broader theoretical approach is needed to account for the use of these various representations to visualize chemical phenomena in the laboratory. In this regard, we draw on situative theory to complement Mayer’s cognitive theory.

In brief, situative theory posits that the physical and social characteristics of a specific setting shape the interpersonal and psychological processes that occur within that setting, including those processes related to understanding and learning (Greeno, 1998; Roth, 1998, 2001; Lave & Wenger, 1991). Characteristics of physical objects in a specific setting enable (i.e., afford) or constrain the way those in that setting talk, think, understand, etc. For example, the availability of chemical reagents in a laboratory affords certain kinds of discussions about the physical properties—color, viscosity, smell, etc.—of the compounds. On the other hand, the physical properties of chemical reagents do not as such facilitate discussions about the composition or structure of the molecules or the processes by which these molecules are transformed, as observed in our ethnographic study of chemistry students (Kozma, 2000b).

Situative theory also emphasizes interactions among individuals as they are engaged in activities within an organized social system. Regular patterns of activities within these systems are characterized as practices of a community. From this perspective, learning occurs as individuals become attuned to the constraints and affordances of the patterned physical and social situations of a community and become more centrally involved in the community’s practices. Through these social interactions within and outside the group, identities and affiliations are formed which influence the motivation to participate in the community’s practices and adopt community standards and norms.

Representations play a particularly important role within the situative theoretical perspective for representations allow the consideration and discussion of objects and processes that are not present or otherwise apparent in a specific situation. Representations—such as written or drawn symbols, iconic gestures or diagrams— “stand for” or “refer to” other objects or situations and thus they become part of the material resources of the current context. It is by the use of these representations that chemists are able to visualize, discuss, and understand the molecules and chemical processes that account for the more perceivable reagents and phenomena they observe in the laboratory. However, the meaning of a representation is not embedded in the representation itself but is assigned to the representation through its use in practice—in the case of chemistry, the use of various chemical symbol systems in the context of laboratory investigations. A crucial part of any social system or community is the conventions of interpreting meanings of representations. As individuals become integrated into a community of practice, they progressively use its representational systems in meaning-making activities. And in turn, representations come to be useful tools for constructing and communicating understanding.

From the situative perspective (Greeno, 1998) classrooms that support investigative practices are ones that encourage students to participate in activities in which representations are used in the formulation and evaluation of conjectures, examples, applications, hypotheses, evidence, conclusions, and arguments. In the subsequent section, we derive implications from our study of chemists' use of representations (Kozma, et al., 2000) for the design of educational experiences in chemistry, if the educational goal is to promote learning by laboratory investigation (Krajcik, et al., 1998). In the section following that, we use both the cognitive and situative perspectives to analyze certain technology applications and studies which examine the use of various visualizations to support students' learning of difficult concepts and principles and their laboratory investigations in chemistry.

New Goals and Resources for Chemical Education

Our comparisons between expert chemists and chemistry students and the learning theories described above have significant implications for chemical curricula and pedagogy. The laboratory practices of chemists suggest that a curriculum based on investigation should not only emphasize the experimental aspects of chemistry but the representational and social aspects, as well. That is, the process of chemical investigation depends not only on experimental procedures but on the social discourse by which the purposes and results of laboratory investigations are represented and understood.

Krajcik and his colleagues (1998) propose a project-based approach to science learning in which students work in pairs or groups to conduct extended investigations in which they pose scientific questions, plan and design investigations and procedures, construct apparatus, carry out their experiments, interpret data, draw conclusions, and present their findings. Discourse is an essential component of such an investigative approach for it is by "talking science" that students come to understand the phenomena that they are investigating (Lemke, 1990). Our analysis of the practices of chemists supports this position. It also supports the central role that visualizations play in scientific meaning making. We have drawn on the findings of our own research in chemistry (Kozma, 2000a, 2000b, 2000c; Kozma, Chin, Russell, & Marx, 2000; Kozma & Russell, 1997) and that of others (Amman & Knorr Cetina, 1990; Chi, Feltovich, & Glaser, 1981; diSessa, et al., 1991; Dunbar, 1997; Glaser & Chi, 1988; Goodwin, 1995; Larkin, 1983; Larkin, McDermott, Simon, & Simon, 1980; Roth, 1998; Woolgar, 1990) to develop a notion of "representational competence" as an important set of skills and practices to be included in the chemistry curriculum (Kozma 2000a)

Representational Competence

Representational competence is a term we use to describe a set of skills and practices that allow a person to reflectively use a variety of representations or visualizations, singly and together, to think about, communicate, and act on chemical phenomena in terms of underlying, aperceptual physical entities and processes (Kozma, 2000a, 2000b; Kozma & Russell, 1997). The act of using representations to successfully construct chemical understanding at once constitutes the meaningfulness of the representation and confirms that the user's ability to participate in this representational, meaning-making activity. While those with little representational competence in a domain rely primarily on the surface features of representations to derive meaning (Chi, Feltovich, & Glaser, 1981; diSessa, et al. 1991; Kozma & Russell, 1997) or the mechanical application of symbolic rules (Krajcik, 1991), those with more skill have come to use a variety of formal and informal representations together to explain phenomena, support claims, solve problems, or make predictions within a community of practice (Amman & Knorr Cetina, 1990; Dunbar, 1997; Goodwin, 1995; Kozma, et al. 2000; Kozma & Russell, 1997; Roth, 1998; Woolgar, 1990).

The performance of chemists in our studies suggests that the following skills might constitute the core of a substantive curriculum of representational competence in chemistry:

- The ability to use representations to describe observable chemical phenomena in terms of underlying molecular entities and processes.
- The ability to generate or select a representation and explain why it is appropriate for a particular purpose.
- The ability to use words to identify and analyze features of a particular representation (such as a peak on a coordinate graph) and patterns of features (such as the behavior of molecules in an animation).
- The ability to describe how different representations might say the same thing in different ways and explain how one representation might say something different or something that cannot be said with another.
- The ability to make connections across different representations, to map features of one type of representation onto those of another (such as mapping a peak of a graph onto a structural diagram), and to explain the relationship between them.
- The ability to take the epistemological position that representations correspond to but are distinct from the phenomena that are observed.
- The ability to use representations and their features in social situations as evidence to support claims, draw inferences, and make predictions about observable chemical phenomena.

We propose a conceptual structure of these skills that organizes them into characteristic patterns of representational use at five stages or levels (see Table 1). This structure corresponds to a developmental trajectory that generally moves from the use of surface features to define phenomena which is characteristic of novices within a domain (Chi, Feltovich, & Glaser, 1981; Glaser & Chi, 1988; Kozma & Russell, 1997; Larkin, 1983; Larkin, McDermont, Simon, & Simon, 1980)—to the rhetorical use of representations, which is characteristic of expert behavior (Amman & Knorr Cetina, 1990; Goodwin, 1995; Dunbar, 1997; Kozma et al., 2000; Woolgar, 1990).

Table 1. Summary of Representational Competence Levels

Level 1: Representation as Depiction

When asked to represent a physical phenomenon, the person generates representations of the phenomenon based only on its physical features. That is, the representation is an isomorphic, iconic depiction of the phenomenon at a point in time.

Level 2: Early Symbolic Skills

When asked to represent a physical phenomenon, the person generates representations of the phenomenon based on its physical features but also includes some symbolic elements to accommodate the limitations of the medium (e.g., use of symbolic elements such as arrows to represent dynamic notions, such as time or motion or an observable cause, in a static medium, such as paper). The person may be familiar with a formal representational system but its use is merely a literal reading of a representation's surface features without regard to syntax and semantics.

Level 3: Syntactic Use of Formal Representations

When asked to represent a physical phenomenon, the person generates representations of the phenomenon based on both observed physical features and unobserved, underlying entities or processes (such as an unobserved cause), even though the representational system may be invented and idiosyncratic and the represented entities or processes may not be scientifically accurate. The person is able to correctly use formal representations but focuses on the syntax of use, rather than the meaning of the representation. Similarly, the person makes connections across two different representations of the same phenomenon based only on syntactic rules or shared surface features, rather than the shared, underlying meaning of the different representations and their features.

Level 4: Semantic Use of Formal Representations

When asked to represent a physical phenomenon, the person correctly uses a formal symbol system to represent underlying, non-observable entities and processes. The person is able to use a formal representational system based on both syntactic rules and meaning, relative to some physical phenomenon that it represents. The person is able to make connections across two different representations or transform one representation to another based on the shared meaning of the different representations and their features. The person can provide a common underlying meaning for several kinds of superficially different representations and transform any given representation into an equivalent representation in another form. The person spontaneously uses representations to explain a phenomenon, solve a problem, or make a prediction..

Level 5: Reflective, Rhetorical Use of Representations

When asked to explain a physical phenomenon, the person uses one or more representations to explain the relationship between physical properties and underlying entities and processes. The person can use specific features of the representation to warrant claims within a social, rhetorical context. He or she can select or construct the representation most appropriate for a particular situation and explain why that representation is more appropriate than another. The person is able to take the epistemological position that we are not able to directly experience certain phenomena and these can be understood only through their representations. Consequently, this understanding is open to interpretation and confidence in an interpretation is increased to the extent that representations can be made to correspond to each other in important ways and these arguments are compelling to others within the community.

There are a number of assumptions embedded in the representational competence structure. First, we assume that the acquisition of these skills follows a developmental trajectory. However, we do not feel that this trajectory is a stage-like, Piagetian progression of personal development (Piaget, 1972). Rather, we ascribe to the Vygotskian notion that development depends on the person's development as well as the physical, symbolic, and social situation (Vygotski, 1980, 1986). Vygotski describes a "zone of proximal development" in which an individual's personal development is supplemented by interactions with the material and social resources in the environment. This position is quite sympathetic with situative theory, with its emphasis on the progressive use of representational conventions to become more centrally involved in a community of practice.

We make no assumption that the development is automatic or uniform. Quite possibly, a person may display behaviors associated with a higher level (say Level 3) in one context and others that are coded at a lower level (Level 2) in another context. Or a person may display a higher level skill on one occasion and a lower level on the same skill at a later time. Also, different levels of development may be displayed with different formal symbol systems or representations. That is, a person may be more competent and show higher level skills with a particular system (say chemical equations) than another (for example, graphs). However, over time and given appropriate sets of physical, symbolic, and social situations, a student will increasingly display more-advanced representational skills, come to internalize these, and integrate these into regular practice.

Pedagogical Activities that Support Representational Competence

The findings of our research and that of others (Roth, 1998; Roth & McGinn, 1998; Bowen, Roth, & McGinn, 1999) suggest that representational skills can best be developed and used within the context of student discourse and scientific investigations. The use of language and representations during the investigative process is also more likely to lead to a deeper understanding of chemical phenomena. Krajcik and his colleagues (Krajcik, Blumenfeld, Marx, Bass, Fredricks, & Soloway, 1998) propose a five-phase approach to structuring student investigation and collaboration. Language and representations can be embedded in each of these phases, as students pose questions, plan, execute, analyze, and discuss their investigations.

- Ask questions: In this phase, students draw on their personal experiences and background knowledge to ask questions, make predictions, and judge the worthwhileness and feasibility of their investigation. Questions and predictions can not only be in verbal form but can use other representations (e.g., "When the reaction reaches equilibrium, the lines of the graph will flatten."). In our ethnographic study (Kozma, et al., 2000), we often saw chemists use molecular diagrams to think through the hypotheses for their experiments.
- Design investigations and plan procedures: Here students design their investigation, decide on what variables to use, design measurements to make, and how they will manage data collection. Language and representations can be used to help students think how the physical experiments that they design can help them understand the chemical processes that underlie the phenomena they observe.
- Construct apparatus and carry out investigations: With this step, students select or build apparatus, make observations, take measurements, and record data. An issue embedded in this phase is how the data should be represented (e.g., As numbers, as a graph, as a diagram? What do you gain or lose with one form or the other?).
- Analyze data and draw conclusions: Students transform, analyze, and interpret data, and use them to draw explanations, arguments, and conclusions. This can involve assigning meaning to a specific feature of a representation (e.g., a peak on a graph) and the coordination of meaning across representations (e.g., that the peak on a graph corresponds to a particular observable event, like a change in color) to help them understand the underlying chemistry.
- Present findings: Finally, students exchange information, share and clarify ideas, give and receive assistance and feedback, create artifacts, and present findings. Again, representation is key here. How do students present their findings in a convincing way that helps others understand the underlying chemistry?

Various visualization technologies can play a key role in supporting investigation and representational practices. As students conduct their investigations, the need to acquire relevant concepts and principles takes on greater salience for them. Representations and visualization technologies can also play a role in this regard, as we saw in our review of Mayer's (2001, 2002, 2003) cognitive theory of multimedia.

Visualizations in Chemical Education

What implications do these findings have for visualizations in chemical education? In the following sections we examine how visualizations fit into the two the complementary theories of learning and understanding. We draw implications from these theories for the use of visualizations in chemical education and use the implications to consider two principal types of chemical visualizations for education: molecular models and simulations and animations.

Molecular Modeling

Gilbert and Boulter (1998) discuss the learning of science through models and modeling. These authors use the term “model” broadly to include representations of ideas, objects, events, processes, or systems. For historical reasons, we use the term here more narrowly. In chemistry, “model” has come to refer to a physical or computational representation of the composition and structure of a molecule and that is how we use the term in this section. In the subsequent section, we refer to representations of systems of molecules as “simulations” or “animations”.

Historically, chemical equations were the earliest representation of molecules and molecular systems. Chemical equations identify the reactants and products of a chemical reaction but they do not show the bonding patterns or geometric structure of molecules. They show conservation of atoms and thus mass in a reaction but do not show the mechanism for the reaction. Structural diagrams are better at showing the geometric arrangement of atoms in the molecule but they do not allow for manipulation of the structure. As mentioned earlier, the development of molecular models—first as physical structures, then as computer representations—allowed chemists to explicitly display and manipulate the geometric structure of molecules (Francoeur, 1997, 2002).

Molecular modeling software allows the chemist to generate and visually display electron density and electrostatic potential surfaces and images of the highest occupied (HOMOs) and lowest unoccupied molecular orbits (LUMOs). This visualization technology is now an essential supplement to the chemical equation for most chemical applications including research, textbooks, and instructional software. Many modeling programs allow the users to construct the molecules from atoms, find the lowest energy geometric structure, measure bond lengths and angles for this structure and manipulate the visualization. Typically, users can rotate the model and look at it from different angles. This supports the laboratory practice of synthesis by allowing chemists to look for reactive sites within molecules and speculate on reaction mechanisms.

Several universities have integrated computational chemistry with extensive molecular modeling experiences throughout their undergraduate curricula (Jones, 2001; Kantardjieff, Hardinger, & Van Willis, 1999; Martin, 1998;Paselk & Zoellner, 2002). Molecular modeling exercises using Spartan or HyperChem have been used as laboratory supplements in introductory chemistry (Cody & Wiser, 2003), organic chemistry (Hessley, 2000), and inorganic chemistry (Montgomery, 2001) or as the basis for entire courses such as structural biochemistry (Dabrowiak, Hatala, and McPike, 2000). Applications of molecular modeling are most common in organic chemistry from simple textbook figures, to Chime-based molecule databases, to animations of reaction mechanisms using ball and stick, space filling, and ball and stick with superimposed HOMOs and LUMOs (Fleming, Hart, and Savage, 2000).

Some authors suggest that molecular modeling visualizations in the form of electron density plots and electrostatic potential surfaces are superior to orbital models for introducing students to molecular structure and bonding (Matta & Gillespie, 2002; Shusterman & Shusterman, 1997). The electron density, _(x,y,z), represents the probability of finding any one of the electrons in a molecule in a small volume element around point (x,y,z). Electron density is often visualized as a cloud of negative charge that varies in density throughout the molecule. Isodensity surfaces of electron density can be displayed to show bonding types and as electrostatic potential surfaces and to probe charge variations over the molecule (see figures in Shusterman & Shusterman, 1997). Electrostatic potential models are useful for investigating intermolecular interactions, identifying reactions sites for electrophilic and nucleophilic reactions, and relative acidities of acids. Both sets of authors suggest that the concept of electron density is easier for students to grasp than the concept of orbitals since orbitals are pure mathematical constructs that cannot be determined by experiments. A further advantage of using electron density models to introduce chemical bonding is its sound theoretical foundation with measurable outputs that do not require modification or replacement in subsequent courses, as students' understanding deepens.

Dori and Barak (2001) showed that even high school students can benefit from the use of molecular models. Israeli high school students who had performed a series of inquiry-based learning tasks using both physical models and computerized molecular modeling had a better understanding of organic compounds than did a control group of students studying the same topics without the modeling learning tasks. The experimental students were better at explaining concepts such as isomerism and most used sketches of ball-and-stick or space-filling models in their explanations. These modeling tasks had developed students' abilities to communicate chemical concepts using appropriate visualizations showing expert-like skills. Use of the modeling tasks also eliminated the gap between students with high and low pre-course knowledge to provide explanations. The control group students were frequently unable to provide explanations with their answers to questions about molecular structures.

With university students Dori, Barak, and Adir (2003) investigated the effect of a single extra credit molecular modeling assignment on performance on the final exam and a special test of chemical visualization and reasoning skills. Of the 215 students who completed the special test as a first week pretest and fourteenth week posttest, 95 volunteered to do the molecular modeling assignment. These students reported spending 5-10 hours drawing structural formulas, building models for an assigned compound such as vitamin A or DDT, displaying and manipulating the models as wire-frame, ball-and-stick, and space-filling forms, and finding the hybridization and electron charge density of each atom. The experimental group had significantly higher scores than the control group on the post-test (_ < 0.001) and final exam (_ < 0.02). Each third of the groups based upon pretest scores showed improvements on the posttest with differences in gains between the experimental and control groups significant for the middle and high thirds. The authors did note that it may be possible that students volunteering for the extra credit assignment were those that worked more throughout the course.

Not only can molecular models facilitate the acquisition of chemical concepts they can support laboratory practice. In our ethnographic study of organic chemistry students (Kozma, 2000b, 2003), we saw how the use of molecular modeling software can dramatically change students thinking and talking in a laboratory course. In addition to observing students as they worked with lab equipment and reagents, we also observed and coded the discourse and behavior of the same students as they used a molecular modeling package (Spartan) in the computer laboratory to construct and analyze the same compound that they had previously synthesized in the wet lab. In contrast to their discourse during the wet lab session, students using the computer modeling software exhibited far more references to chemical concepts, such as atoms, bonds, electronegativity, dipole moment, and so on. Student discourse while using modeling software was much more like that of laboratory chemists in our study (Kozma, et al., 2000) than was their discourse in the wet lab. Furthermore, the laboratory instructors were more likely to discuss chemical concepts with students than they were in the wet lab.

Computer Simulations and Animations

While we use the term molecular model to refer to visualizations of individual molecules, we use the terms "simulation" or "animation" to refer to representations of dynamic chemical processes or systems. Simulations allow users to select values for input variables from within suitable ranges and observe the results on output variables. With chemical simulations, users might change pressures in a gaseous system or concentrations of regents in a solution system and observe the impact of these changes on the species in the system. Simulations can be used to explore chemical systems or processes in order to derive or test possible underlying explanations or theoretical models. Gilbert and Boulter (1998) refer to these uses as "exploratory" applications. Three examples of chemical simulations involve concepts related to kinetics (Allendoerfer, 2002), equilibrium (Paiva, Gil, & Correia, 2002) and acid-base titrations (Papadopoulos & Limniou, 2003). All three simulations can be used to not only explore fundamental chemical concepts but to supplement laboratory experiments either as pre-laboratory exercises or as extensions to hands-on laboratories. All these simulations along with several others are included on the General Chemistry Collection, 7th Edition, CD-ROM (Holmes & Gettys, 2003) available from *Journal of Chemical Education Software*.

Chemical animations are dynamic, molecular-level (sometimes referred to as "nano-level" or "nanoscopic-level") representations of chemical systems as they change and their species react. These displays often consist of individual balls or dots, or clusters of these, that represent individual molecules that move about, collide, and react. The results or outputs of simulations are often displayed as animations. However, other simulations (for example, Schoenfeld-Tacher, 2000) represent the simulated experiments with icons that correspond to the experimental apparatus, reagents, instrument readouts, and observable results of experiments, much as they would appear in the wet lab. While animations can represent the outputs of simulations, they can also be mere "canned" movies that illustrate a particular concept at a molecular level without allowing users to manipulate variables.

Most research studies that have been conducted in this area have used animations as movies that illustrate specific concepts, rather than as the output of simulations of chemical systems that student explore. For example, Yang, Greenbowe, and Andre (2004) used molecular-level animations of oxidation-reduction reactions and the movement of ions and electrons in dry cell batteries in flashlight circuits in a tutorial designed to teach concepts about electrochemical cells, such as the movement of electrons between electrodes within the cell, and about electric circuits, in order to overcome such common misconceptions as a decrease in current as electrons flow through a light bulb. An experimental group of volunteers attended an instructor-guided tutorial session rather than the lecture on electrochemical cells. These students, guided by the instructor and worksheets, used the animation software to study the chemical and physical processes occurring in a common flashlight. These animations allowed users to zoom-in to view the processes at each battery electrode separately and to pause, continue, and to replay each animation. Students using the tutorial rather than attending the lecture were more likely (80% versus 57%) to identify the carbon electrode as an inert electrode on the posttest. This study shows the effectiveness of well-designed animations enhancing student understanding of chemical concepts, although the study design confounded the use of animations with the use of tutorials.

In another study, animation and instructional approach were disentangled. Sanger and Greenbowe (2000) examined the impact of animations and conceptual change strategies on students' conceptions of current flow in electrolyte solutions. In this 2 X 2 design, university students in one group received a lecture along with an animation accompanied by lecturer's narration showing the electrochemical processes occurring in a galvanic cell at the nanoscopic level with a focus on the chemical half-reactions occurring at each electrode and the transfer of ions through a salt bridge. Students in the other lecture section saw only static chalkboard drawings of the process. Half the students in these groups also received a conceptual change strategy that confronted typical misconceptions while the other half did not. Students were tested using algorithmic, visual, and verbal test items on both an immediate and a delayed post test. There were no significant differences between any of the treatment and control groups on the algorithmic or visual test items. There was, however, a main effect in favor of the conceptual change strategy (but not one for the use of animations) on the verbal items on both the immediate and delayed post-tests. There was also an interaction between the animation and conceptual change treatments for these items on the immediate post-test such that students who did not receive the conceptual change strategies scored higher with the animations than those students who received the conceptual change strategies but not the animations.

In an experiment by Sanger, Phelps, and Fienhold (2000), students in the treatment group viewed an animation accompanied by narration that showed representations at both macroscopic (i.e., a can being heated, sealed, and crushed upon cooling) and nanoscopic levels (i.e., numbers of 2-D balls representing molecules moving around both inside and outside the can, more quickly or slowly). Students in both the treatment group and the control group received a lecture on gas behavior and observed a physical demonstration of the can-crushing experiment. Students in the treatment group scored significantly higher on measures related to understanding a similar demonstration. In another experimental study (Sanger & Badger, 2001), students in the treatment group received instruction on and demonstrations of miscibility of polar, non-polar, and ionic compounds supplemented by both molecular-level animations of inter-molecular attractions, as well as shaded 2-D pictures of electron density plots ("eplots") that used color to show the polar (i.e., charged) regions of various molecules. Students in the control group received only instruction and demonstrations. Students in the treatment group scored significantly higher on an experimenter-constructed test in which students were asked to identify polar molecules not discussed in the instruction, make predictions about the miscibility of compounds, and explain their answers.

Williamson and Abraham (1995) investigated the use of animations of properties of states of matter and chemical reactions with a quasi-experimental, posttest control-group design. They compared a control group of college students who attended lectures using only static visualizations for these topics with two experimental groups that also used a total of 13 animations of nanoscale properties each with one to two minute durations in lectures. One of the experimental groups also used the animations in their recitation sections held in a computer lab. All groups received the same series of 10 lectures on concepts related to gases, liquids, solids, and solution reactions. Conceptual understanding was measured using the Particulate Nature of Matter Evaluation Test (PNMET) (Williamson, 1992). Students in the experimental groups had mean scores one half a standard deviation above those in the control group on the PNMET. All three groups were equivalent on course achievement, as measured by an hour exam and final exam. Williamson and Abraham suggest that use of animations may increase conceptual understanding by prompting formation of dynamic mental models of the phenomena.

Also at the college level, we (Kozma, Russell, Jones, Marx, & Davis, 1996) examined the impact of a software environment (described in Russell & Kozma, 1994, and in the next chapter) in which students conducted simulated experiments using multiple representations. In this study, students changed variables related to pressure, concentration, and temperature and examined the effect of these changes on the relative concentrations of species in gas-phase and solution equilibrium systems, as represented in video of the experiments, dynamic graphs, and molecular level animations. In this quasi-experimental design, students significantly increased their understanding of concepts related to equilibrium and reduced the number of common misconceptions.

Animations and simulations can also be used to support laboratory practice. Schoenfeld-Tacher, Jones, and Persichitte (2001) used simulations of a virtual laboratory experience as part of a goal-based scenario (GBS) exercise in biochemistry in a study to determine the relationships of cognitive and demographic variable on learning outcomes. This was a macro-level simulation of actual laboratory activities rather than a nanoscale simulation, as those discussed above. Schank, Fano, Bell, and Jona (1993, p. 304) state, "Goal-Based Scenarios are problems in the domain of a student's interest that present definable goals and encourage learning in service of achieving those goals. A GBS is a type of learn-by-doing task with very specific constraints on the selection of material to be taught, the goals the student will pursue, the environment in which the student will work, the task the student will perform, and the resources that are made available to the student." Students in the Schoenfeld-Tacher, Jones, and Persichitte study (2001)used *Whodunnit?* (Schoenfeld-Tacher, 2000), a virtual crime lab that uses DNA fingerprinting techniques to identify a murderer. A pre- and posttest design was used with an experimental group of 458 students in seven sections of biochemistry at three universities and a community college. Results were compared with a 37 person pseudo-control group at one university. The entire *Whodunnit?* GBS was completed in 1-1.5 hours, although there was no indication of how long the simulated laboratory experience took. The control group performed a standard DNA laboratory activity rather than the GBS. A paired comparison t test was used to demonstrate a significant difference between pre- and posttest scores for the experimental group on a multiple choice test measuring knowledge of material presented in the simulation. There were no pre-post differences for the control group. Four demographic variables were studied (gender, race, final course score, and prior science coursework). Only the number or prior science courses in high school showed a significant correlation with learning outcomes. Logical thinking ability but not spatial ability or disembedding ability was related to learning outcomes. This GBS experience with its simulated laboratory appeared to be equally effective for all types of students.

In an application of visualization technology that Gilbert and Boulter (1998) refer to as "expressive", Schank and Kozma (2002) describe a software package called *ChemSense* that allows students to construct molecular-level animations of chemical systems (see also the Russell & Kozma chapter for more description and an example screen shot). While animations were not among the representations that we saw in our observation of laboratory chemists (Kozma, et al., 2000), the assumption behind *ChemSense* is that by enabling students to represent the dynamic, molecular nature of the reactions that they are investigating, the software will support their investigative practices and their chemical discourse about the physical phenomena they observe in the laboratory. In a study of high school students (Michalchik, Rosenquist, Kozma, Schank, & Coppola, 2004), we observed that students used *ChemSense* in the wet lab to move their discourse from a focus on the physical characteristics of their experiments to an analysis of the molecular entities and processes that accounted for physical characteristics and to think more deeply about chemical concepts related to chemical geometry and connectivity. Students came to use the *ChemSense* representations that they constructed as rhetorical artifacts in their discussions with each other and with the teacher. In addition, we found that over the two week-long unit, students significantly improved their scores on measures of both chemical understanding and representational competence (see a discussion of this measure in the Russell & Kozma chapter).

Conclusions and Recommendations

For Instruction

Molecular models, simulations, and animations can support both the traditional concept building goals of the chemistry curriculum, as well as new investigative practice goals; although far more research has been done on the former than the latter. Studies have shown that students can use models to understand concepts related to bonding and structure. They can also support students' laboratory practices, shifting their discussions from the physical aspects of the experiments that they conduct to the chemical entities that underlie these physical phenomena. We saw that animations can help students understand difficult concepts related to equilibrium, electrochemistry, and solution chemistry. They can also be used by students to support their laboratory investigations by helping students discuss their experiments in terms of molecular entities and dynamic processes.

We recommend the widespread us of these visualization resources in chemical education. We particularly recommend the expressive use of visualizations to help students acquire the representational competencies and laboratory practices of chemists.

For Research

Much more research is needed on the impact of visualizations on student learning. Classroom research of the sort we examined is important in order to establish the external validity of the findings on visualizations—that they work in real classroom situations. But there is also a need for carefully controlled experiments in the cognitive laboratory that supplement these classroom studies. For example, some of Mayer's design principles were not tested in several studies because the narration was not included as part of the software presentation and verbal information came from the lecturers. Carefully controlled experiments are needed to confirm the effectiveness of the Mayer principles in chemistry.

Additional classroom studies could examine the effectiveness of these visualizations for different topics or different student groups. For example, more classroom research needs to be done on the use of students' manipulation of simulations of chemical systems. Additional work needs to be done on animations. Are they best for concepts that involve dynamic processes, such as acid-base reactions and oxidation? Are they at all useful for less-dynamic concepts such as molecular structure or is this concept best taught with molecular models? Are animations or simulations useful for analyzing aggregation effects in systems of large numbers?

There is also a significant need for research that focuses on the process of laboratory investigation and how it is that the use of various symbol systems and multimedia environments facilitates investigative practices. There is a need to extend research beyond the lecture hall or computer lab into the chemistry laboratory. New assessments must be designed and used that measure investigation practices and related skills, such as visualization skills or representational competence and these are discussed in the next chapter. Finally, in order to integrate traditional and new curricular goals in chemistry, research studies must examine the relationship between learning investigative practices and the development of chemical understanding and how visualization technologies can facilitate this relationship.

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