Promoting Conceptual Understanding of Chemical Representations: Students' Use of a Visualization Tool in the Classroom

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Abstract: This study investigates how students develop their understanding of chemical representations with the aid of a visualizing tool, eChem, that allows them to build molecular models and view multiple representations simultaneously. Multiple sources of data were collected with the participation of 71 eleventh graders in a high school over a six-week period. The results of the pre- and post-tests show that students' understanding of chemical representations improved substantially (t=13.9, p<.001, effect size = 2.68). The analysis of video recordings reveals that several features in eChem helped students construct models and translate representations. Evidence also shows that high engagement students' discussions involved both visual and conceptual aspects of representations, which in turn deepened their understandings of representations. Moreover, the findings suggest that models can serve as a vehicle for students to generate mental images, and that different types of 3D models were not used interchangeably for these students.

Keywords: chemistry, representation, visualization

Introduction

Students' conceptual understanding of chemical representations is a prominent area of research in chemistry education (Ben-Zvi, Eylon, & Silberstein, 1988; Gabel, 1998). For decades, researchers and chemistry educators have been discussing the three levels of representations in chemistry: macroscopic, microscopic, and symbolic levels (Gabel, Samuel, & Hunn, 1987; Gabel, 1998). Chemical representations at the macroscopic level refer to observable phenomena, such as the change of matter. The microscopic chemistry refers to the nature, arrangement, and motion of molecules used to explain properties of compounds or natural phenomena. Chemistry at the symbolic level refers to the symbolic representations of atoms, molecules, and compounds, such as chemical symbols, formulas, and structures. Empirical studies (e.g. Ben-Zvi, Eylon, & Silberstein 1986, 1987) have shown that learning microscopic and symbolic representations is especially difficult for students because these representations are invisible and abstract while students' understanding of chemistry relies heavily on sensory information.

To help students understand chemistry at the three levels, researchers developed new approaches to teaching chemistry such as adapting teaching strategies based on the conceptual change model, presenting the historical change of a theory, using concrete models, and using technological tools (for reviews, see Gabel, 1998; Krajcik, 1991). For instance, multimedia tools, which integrate the animation of molecular models, video clips of chemical equilibrium, or real time graphics, provide students with opportunities to visualize chemical processes at the microscopic level. According to empirical findings of their studies, Kozma and his colleagues (Kozma, 1997; Kozma, Chin, Russell, & Marx, 1997; Kozma et al., 1996) stated that the use of multiple linked representations helped students understand chemical equilibrium and its related chemical concepts. Additionally, research supports the advantages of manipulating physical models that help students to visualize atoms and molecules and promote long-term understanding (Barnea & Dori, 1996; Copolo & Hounshell, 1995; Gabel & Sherwood, 1980; Talley, 1973).

While empirical studies assert the value of using models and technological tools for chemistry learning, however, little is understood about how models actually support students' learning, how students' use of these models evolve over time in classroom settings, and what features of a technological tool help students to develop conceptual understanding of chemical representations. Moreover, although many professional visualizing tools have been used and developed in chemistry, such as CAChe (Crouch, Holden, & Samet, 1996), none of them were designed for novice users at the high school level. Therefore, the purpose of this study is to deepen our understanding of how high school students develop their understanding of chemical representations by the use of a technological tool with similarities to professional tools, but designed for learners.

The visualizing tool used in this study, eChem, is designed to play a central mediating role by allowing students to build molecular models and view multiple representations simultaneously. This study explores how, with the aid of eChem, students develop their ability to visualize chemical representations, whether they are able to make translations between these representations, and what supports their ability to do so. Two questions guide this study: 1) Are students able to translate between two-dimensional and three-dimensional representations? If so, in what ways does eChem help students translate between representations in chemistry? 2) What learning patterns (e.g., common errors students make while making translations and constructing models, learning strategies they use to translate representations, and commonly used models for their final presentations) do students demonstrate while translating chemical representations and constructing models by using eChem? How do these patterns reveal students' development of conceptual understanding of chemical representations?

In order to investigate how students develop understanding of chemical representations with the use of eChem in classroom settings, this study was conducted in a natural classroom context and did not involve a control group. Because a learning environment involves various factors influencing students' learning, such as teacher's pedagogical content knowledge and collaboration between students, the learning effects caused by the use of eChem or by the contribution of other factors are inseparable. Additionally, the data for this study were collected in a project-based science classroom (Blumenfeld, Marx, Patrick, Soloway, & Krajcik, 1995; Marx, Blumenfeld, Krajcik, & Soloway, 1997). Thus, the findings and results could not be generalized to a lecture-oriented science classroom.

Theoretical background

Chemistry and Representations

As applied theoretical and physical chemists, Hoffman and Laszlo (1991) claimed that representations in chemistry are metaphors, models, and theoretical constructs of chemists' interpretation of nature and reality. Chemical representations in this study refer to various types of formulas, structures and symbols used in chemistry. The drawing of molecular structures and the writing of chemical formula are "ideology-laden" and "theory-laden" (Hoffmann & Laszlo, 1991) that convey messages of the development of chemical theories and experiments. Chemical representations thus are meaning-based knowledge representations, which are changed and created to reflect the reunification or reconstruction of the theoretical and the experimental.

Additionally, representations in chemistry share following characteristics. First, representations in chemistry are models suitable for specific purposes (Hoffmann & Laszlo, 1991). For example, ball-and-stick models represent the physical positions of atoms and molecules, and space-filling models provides information about the size of atoms that is critical for deciding the conformation of organic molecules. Hence, representations embed selected details of the relevant concepts or principles, but permit other details to fade. Second, the development of representations displays the historical development of theories in this domain. By examining the evolution of the chemists' way of seeing and drawing, Hoffmann and Laszlo stated:

> It [Chemistry] has shed to a large extent its childhood habit of going no further than a phenomenological description of bulk properties, at the macroscopic level…Chemistry has become a microscopic science. Explanations nowadays go routinely, paradigmatically from the microscopic scale to the observable; from the way the electrons are distributed in a dye molecule to its color; from the detailed shape of a molecule and of the electrostatic potential around it to its pharmacological activity. (Hoffmann & Laszlo, 1991, p. 8)

That is, microscopic representations currently used in chemistry evolve from phenomenological analogies of sensory experiences at the macroscopic level. Because these microscopic representations are historically developed and have been extracted from the observable phenomena, understanding these representations becomes a difficult task. For novices, these representations cannot be understood by personal intuition or perceptions. Consistent with this historical development, Gabel, Samuel and Hunn (1987) indicated that most chemistry concepts have three levels of understanding: the sensory, particulate, and symbolic levels. Chemists transform the sensory information into chemical processes, explain these processes as atomic and molecular behaviors at the particulate level, and translate atoms and molecules into symbols and formulas. As we will discuss later, this abstract nature of representations is one source of students' learning difficulties.

Third, representations in chemistry are symbols, signs or elements of chemical language and vehicles for viewing the world (Hoffmann & Laszlo, 1991; Kozma et al., 1997; Kozma, 1997). Hoffmann and Laszlo (1991) argued that "a chemical formula is like a word" which composes the language of chemistry and "purports to identify, to single out the chemical species it stands for." The most important implication of this analogy is that both language and chemical representations share the function of communication. In their ethnographic study at a chemistry laboratory, Kozma, Chin, Russell and Marx (1997) found that chemists used representations to communicate with each other and reconstructed reality and nature. They used various representations for asking questions, stating hypotheses, making claims, drawing inferences, and reaching conclusions. Being familiar with these representations and their usage in chemistry, therefore, is essential for the acquisition of expertise. As Kozma indicated (Kozma, 1997), "the use and understanding of a range of representations is not only a significant part of what chemists do—in a profound sense it *is* chemistry" (original emphasis). Thus, Kozma and Russell (1997) suggested that chemistry education should promote students to develop "representation competence." The competence comprises a set of representational skills: the ability to see expressions with different surface features (e.g., changes in color), as representing the same chemical principle or situation, the ability to translate one representation of a chemical concept or situation into another one, and the ability to generate or select an appropriate representations to make explanation, predictions, and justification. Namely, representation competence includes the abilities and skills to use a range of chemical representations to do chemistry inquiry.

In sum, representations are theory-laden models and chemists' interpretations of nature. Each type of representations conveys information about some relevant concepts but fade other details. Further, the usage of representations in chemistry reflects the theories, findings and discoveries in chemistry. Representations are the elements of chemistry language; chemists use them to communicate with their colleagues and to do inquiry. The acquisition of the expertise in the chemistry domain would be the development of "representation competence." Chemistry education should help students learn how to use representation appropriately. While representations play a critical role in chemistry, however, the literature indicates that many students have difficulty visualizing these representations. Because most students' understanding of chemistry is constrained by the perceptual experiences from daily lives, students tend to stay in the sensory level and are not able to visualize particulate behavior and symbolic representations (e.g., Ben-Zvi, Eylon, & Silberstein, 1986; Gabel et al., 1987).

Students' Learning Difficulties

In Ben-Zvi, Eylon, and Silberstein's study (1988), they explored what level of descriptions students generated (e.g., the macroscopic level, the atomic molecular level, the multi-atomic level), when some chemical symbols and formulas were used, such as $Cu_{(s)}$, $H_2O_{(l)}$, and $Cl_{2(g)}$. Students' responses indicated that a majority of them confused atoms with molecules. Although most of them generated some macroscopic descriptions of water, i.e., its properties, the atomic-molecular models they used to explain the phenomena were not appropriate. For example, about 20 percent of the students in their study held an additive model of molecules and stated that a water molecule contained a unit of hydrogen gas, H_2. Some students viewed $H_2O_{(l)}$, and $Cl_{2(g)}$ as representations of one particle without the conception of atoms or a collection. To them, the use of (l) or (g) could not trigger any descriptions about multitude of molecules. Ben-Zvi et al. also found that even though most students were able to recognize these chemical symbols as hydrogen or chlorine, they relied on their intuitive mental models of atoms and molecules to make explanations or descriptions about these representations. Many students, even after studying chemistry, do not understand the role of a formula; some think that formulas are merely abbreviations for names rather than a short way to represent composition or structure and others hold the misconception that a formula is an abbreviation for a mixture.

Moreover, most students have difficulties interpreting chemical equations, because their understanding is constrained by the surface features of representations (Kozma & Russell, 1997; Krajcik, 1991). When they see an equation, such as $C_{(s)} + O_{2(g)} \rightarrow CO_{2(g)}$, they interpret it as a composition of letters, numbers and lines rather than a process of bond formation and breaking. The technique of balancing chemical equations makes them picture chemical equations as mathematical puzzles (Ben-Zvi et al., 1987), and they can even work algorithmic without having a conceptual understanding of the phenomena. Thus, while chemists see symbols and letters as molecules and the arrow as the direction of reaction, many students are not able to visualize these representations.

In addition to the difficulty of interpreting representations, Keig and Rubba's study (1993) showed that large numbers of students were unable to make translation among formula, electron configuration, and ball-and-stick models. Compared with chemists, students are less capable to providing equivalent representations and verbal descriptions for a given representation (Kozma & Russell, 1997). Hence, the present study focuses on how students learn to interpret molecular and symbolic representations and make translations among them.

The literature suggests that two aspects of chemical representations cause these difficulties. First, representations, especially symbolic and molecular ones, are abstract and cannot be understood by intuition (Ben-Zvi, Eylon, & Silberstein, 1988). It has been known that meaningful learning is built on a relevant set of concepts already held by the student. Without explicit connections between phenomena and representations, students cannot assimilate these new knowledge elements into their cognitive framework. Therefore, to make these representations understandable and meaningful for students, instruction, technological tools or chemistry curriculum should give students opportunities to build conceptual connections between these abstract molecular symbols and collective behaviors of molecules. Next, students' ability to visualize representations is correlated to their understanding of the underlying concepts (Keig & Rubba, 1993). For example, considering the translation between the chemical formula of water (H_2O) and its structural formula, we are unable to draw a chemically correct structure unless we have the conceptual understanding of covalent bonds and the shapes of molecules. To translate the formula into a structure, we need to identify that each hydrogen atom has one single bond, since it has only one valence electron to share with an oxygen atom. Then the understanding of unshared electron pairs assists us to decide the shape of the molecule. The formula, H_2O, explicitly conveys the identity of the constituent elements and their ratio, but does not indicate the bond angle or whether the bonds are single or double. Thus, translation between representations is an information processing task, requiring understanding of the underlying concept to the extent that the individual can interpret the information provided by the initial representation and infer the details required to construct the target representation (Keig & Rubba, 1993).

Lesh, Post and Behr (1987) further illustrated the information processing character of translation among representations, and the role of concept knowledge in the translation process. Each student's knowledge of representations in terms of atoms and molecules provides a foundation for translation of representations. This foundation is more like a network for the cognitive application of connections or relationships between these concepts. According to Keig and Rubba's empirical study (1993), students' performances on the translation of representations were not correlated to reasoning ability, spatial reasoning ability and gender but the specific knowledge of the representations. Their findings suggested that concepts established in the student's mind enabled the creation of connections and relationships between those concepts that, in turn, provided the cognitive structures to support the cognitive processing tasks. When external representations trigger the nodes of this cognition network, the relevant concepts connected to these nodes are activated to complete the translation process (Gagne, Yekovich, & Yekovich, 1993). Without appropriate understanding of underlying concepts, most students are not capable to translate from a given representation to another one.

Consequently, making conceptual connections between representations and developing understanding of underlying concepts are important for students to learn chemistry. Various effective teaching strategies based on the conceptual change model have been discussed (e.g., Gabel, 1998; Krajcik, 1991) to foster students' learning. To focus on the research questions, we will not discuss how to help students learn representations from a pedagogical perspective but review the literature about using models and tools in the classroom.

The Use of Molecular Models and Technological Tools

In order to ease students' learning difficulties of chemical representations, various learning strategies are suggested. The increased use of physical or computational models is striving to achieve this goal. Copolo and Hounshell (1995) compared the learning effects of using two- and three-dimensional model representations of molecular structures on student learning of organic chemical structures. In their study, organic structures were taught to high school students using one of four methods of molecular representations: (1) two-dimensional (2D) textbook representations, (2) three-dimensional (3D) computer models, (3) three-dimensional ball-and-stick models, and (4) combination of the computer molecular models and the ball-and-stick models. The students in the combination group, using both computer and ball and stick models, scored significantly higher on the retention test compared to the other groups. This result is consistent with Gabel and Sherwood's finding (1980) that manipulating physical models offered the "long-term cumulative effects of students' understanding." Thus Copolo and Hounshell concluded that both the physical and computational models could offer benefits as an effective tool for teaching molecular structures and isomers. They also noted that "students need assistance with mental transference from three dimensions to two dimensions," so instruction should include both forms of representation to guide students in making the mental transfers. Yet, this experimental study did not provide qualitative data to examine how students developed understanding of chemical representations over time and what features of computational models supported students' learning.

In order to explore students' use of atomic and molecular models in leaning chemistry and to realize the power of models as aids to learning, O'Connor (1997) conducted a qualitative study in general chemistry courses at two colleges. According to the findings, she suggested that the instructors "must give much attention to the selection, use, integration, and limitations of models," since, despite extensive exposure to models in lectures, textbooks and the computer-based activities, the college students in her study still used surface/visual features of models to construct their explanation and overlooked the relevant concepts underlying models. Heavy reliance on the surface features to categorize representations and to solve problems is a significant characteristic of novices in science domains (Chi & Feltovich, 1981; Kozma & Russell, 1997). Whereas O'Connor's study with the sample of college students provided educational implications about how to use models in the classroom, it did not inform us how high school students, as novices with relatively limited knowledge of molecular representations, learned to use these models and understand relevant concepts. Additionally, it did not provide evidence of how computational models could be beneficial for students.

Kozma and his colleagues (Kozma, 1997; Kozma, Chin, Russell, & Marx, 1997; Kozma et al., 1996) found that the use of multiple, linked representations helped students understand chemical equilibrium and its related chemical concepts. The multimedia environment named MultiMedia and Mental Models (4M:Chem) integrated four chemical systems about equilibrium. It was designed to make the symbolic elements correspond to features of real world, connect to graph representations, and integrate conceptual entities and expert-like mental models (Kozma et al., 1996). Kozma et al. provided insights into how multimedia integrated multiple chemical representations and how symbol elements interacted with students' mental models. However, the well-designed tool (4M:Chem) did not give students opportunities to create artifacts or externalize their understanding. All videos, graphs and animations were already built in, and students could not change or create any representations to meet their learning needs.

With rapid development of Internet technology, more and more molecular modeling tools can be downloaded from the web. The Chime[1] plug-in makes commercial browsers (Netscape® navigator or Microsoft® Explorer) display two-dimensional (2D) or three-dimensional (3D) molecules within a web page. TINKER-molecular modeling software is a computational package for molecular mechanics and dynamics with special features for protein molecules (http://dasher.wustl.edu/tinker). It includes a variety of novel algorithms and parameter sets for computing polarizablity and surface area. RasMol (http://www.umass.edu/microbio/rasmol) is molecular visualization freeware. It allows students to rotate 3D molecules, but all these molecule files for rotation need to be downloaded in advance. MathMol (http://www.nyu.edu/pages/mathmol) combines mathematics and chemistry and proposes to provide students and teachers with basic concepts in mathematics and their connections to molecular modeling. As other professional visualizing tools (e.g., CAChe), however, these programs are designed for college students or chemists. For high school students, as novices in chemistry, these tools are difficulty to learn and use. Complicated calculations and parameters, including bond length, bond angle, and vibration energy, are overwhelming and students need to memorize programming language or commands to use some of them.

Therefore, whereas many professional visualizing tools have been used and developed in chemistry, none of them were designed for novice users at the high school level. One objective of this study is to investigate how high school students develop the understanding of chemical representations by the use of a technological tool with similarities to professional tools. Additionally, although most empirical studies have shown positive results of using models for chemistry learning at the high school and college levels (Barnea & Dori, 1996; Copolo & Hounshell, 1995; Gabel & Sherwood, 1980; Talley, 1973), the learning issues in terms of how to use models in the real

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[1] Chime version 2.0a for Macintosh PowerPC, Copyright (c) 1996-1998 MDL Information Systems, INC.

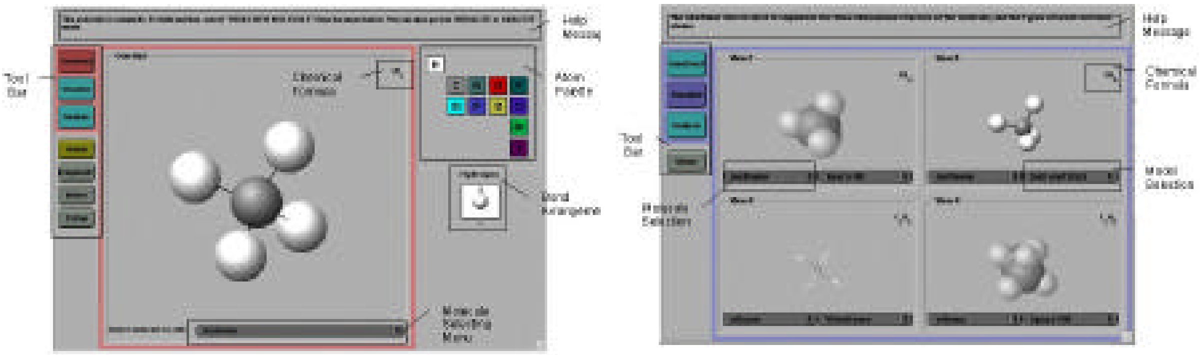
classroom context should not be oversimplified. As Haidar and Abraham (1991) stated, “this abstract relationship between model and reality requires science educators to help in the development of students’ reasoning abilities in order to be able to make the line between model and reality.” For high school students, making connections between chemical representations and observable phenomena is not an automatic mental process as it is for chemists. Thus, this study attempts to address how students use molecular models to learn chemical representations and to explore what aspects or features of a technological tool support them to do so.

Technological tool—eChem

The technological tool used for this study was eChem, a simplified and learner-centered version of professional visualizing tools, developed by the Center for Highly Interactive Computing in Education (hi-ce) at University of Michigan. Learner-centered design (LCD) addresses the unique needs of learners (Jackson, Krajcik, & Soloway, 1998). The principles of learner-centered design support acquisition and growth of expertise, address diversity of learners’ background, and promote and sustain motivation.

eChem guides students in three main actions—building molecules, visualizing multiple 3D models, and comparing micro- and macroscopic representations. eChem provides three tasks: *Construct*, *Visualize* and *Analyze*. In *Construct*, students can create organic molecular structures, view them from all possible angles, and manipulate them more easily than physical ball-and-stick models (see Fig. 1(A)). *Visualize* provides students with multiple views of different compounds and various representations such as ball-and-stick, wire-frame and space-fill simultaneously (see Fig. 1(B)). In *Analyze*, students can make connections between molecular models at the microscopic level (molecular structures) and their collective behaviors at the macroscopic level (chemical and physical properties).

As shown in Table 1, eChem provides various supports for chemistry learning. To support the acquisition of expertise for high school learners, eChem simplifies the periodic table to an atom palette (Fig. 1). Rather than providing the full scope of chemical bonding, constraining the scope to organic and covalent compounds simplifies the learning process, lowers the cognitive burden, and makes molecular models more understandable for novice users. Further, eChem provides only possible bonding arrangements (hybridization) to support learners to create appropriate chemical models. Although the number of bonding arrangements is limited, complicated molecular models are still doable in eChem. For example, with the growth of expertise, students can use eChem to construct complex molecules such as glucose, DDT (DichloroDiphenyl Trichloroethane), or fatty acids. Additionally, when students choose and switch between different actions and features, eChem provides Help messages (Fig. 1) to support their learning and using process.



(A) (B)

Figure 1. (A) The graphic interface of *Construct* page and (B) the graphic interface of *Visualize* page

Table 1. Learning supports provided by eChem on the three tasks.

Learning supports	**Construct**	**Visualize**	**Analyze**
Growth of Expertise			
Multiple linked representations	· Chemical name (S), formula (S), ball-and-stick models (MI)	· Chemical name (S), formula (S), various 3D models (e.g., ball-and-stick, wire-frame, space-filling models)(MI)	· Chemical name (S), ball-and-stick model (MI), property (MA)
Reduce complexity	· Simplified periodic table · Limited bond arrangements · Model rotation	· Select molecules · Select models · Model rotation	· Select molecules · Spread sheet of structures and properties · Model rotation
Explicit guidance	· Help message	· Help message	· Help message
Diversity of learners			
Multiple representations	· Chemical name (S) · Chemical formula (S) · Ball-and-stick model (MI)	· Chemical name (S) · Chemical formula (S) · Multiple 3D representations (MI)	· Chemical name (S) · Ball-and-stick model (MI) · Property (MA)
Non-linear path	· Tool bar · Graphic interface	· Tool bar · Graphic interface	· Tool bar · Graphic interface
Motivation			
Visual engagement	· Graphic interface	· Graphic interface	· Graphic interface
Sustain engagement	· Revised models · Molecule database		· Property database

MA: macroscopic representation MI: microscopic representation S: symbolic representation

To address diversity of learner's background and facilitate visual engagement, eChem's visual interface supports a non-linear path to construct, visualize and analyze molecular models. Students can switch between actions and features easily by clicking buttons on the tool bar. Its multiple linked representations allow students with different learning styles to choose their preferred symbol systems (Salomon, 1979) and foster them to make connections between verbal and visual representations simultaneously (Clark & Paivio, 1991). Furthermore, compared with the built-in multimedia software which has a limited number of molecules to manipulate, eChem allows students to revise their models and create their own database of compounds over time.

Methods

Context

This study was conducted in a small public high school in an urban university town in the Midwest. The teachers in the science program worked with educational researchers from a local university to develop and implement a three-year, project-based science curriculum (Marx, Blumenfeld, Krajcik, & Soloway, 1997). Seventy-one eleventh graders in three sections participated (n=71, 35 females) and were taught by three different teachers. The students in this study had a range of ethnic backgrounds, academic abilities, and socioeconomic levels, although the majority of students were white, middle- to upper middle-class.

The use of the tool, eChem, was integrated into a six-week project called the Toxin Project. In this project, students worked in small groups and selected a known toxin to investigate from a list provided by the teachers. The driving question of this project was “Is my drinking water safe?” To answer this question, students were lectured on relevant chemical concepts, searched for information from the web, watched videos of water treatment and environmental science, carried out lab activities of solubility and water purification, built physical and eChem models, and designed webpage for final products.

From week 2 to week 4, students used three learning activities that incorporated the main actions of eChem to study hydrocarbons and alkanes (eChem I), names of alkanes (eChem II), and representations of chemistry (eChem III). The first eChem activity, tied to a lecture on covalent bonds, introduced structures and properties of organic compounds. Students constructed models of alkanes, viewed various representations simultaneously, and developed the relationship between boiling points of alkanes and the number of carbons. The second activity introduced IUPAC (International Union of Pure and Applied Chemistry) nomenclature of organic compounds, the naming rules currently used in chemistry. Students created models on eChem and followed the rules to name their models. The third activity was designed for students to visualize various two-dimensional (2D) and three-dimensional (3D) chemical representations. The 2D representations included structural formulas, condensed structural formulas, very condensed structural formulas, and chemical formulas. The 3D models constructed in this activity included the ball-and-stick, space-filling and wire-frame models. Students constructed models using eChem and ball-and-stick kits and compared differences and similarities between these two types of models.

Data collection

Multiple sources of data were collected over a six week period. Curriculum materials, classroom videos, and field notes of classroom observations were collected to describe the implementation of the curriculum. All participants (n=71, 35 females) took pre- and post-tests. Twenty-one items were grouped into three types of conceptual understandings: 1) chemical representations, 2) chemical concepts underlying representations, and 3) connections between properties and molecular structures. Students were asked to make 2D and 3D translation, compare structural differences based on 2D structural formulas, identify types of bonding based on chemical formulas, and determine the polarity of molecules by structures. In addition, video recordings while students used eChem (process videos), students’ artifacts, and interview data were collected from eighteen target students (three pairs in each section). Process videos captured activities on a computer screen and conversations of target groups. Students’ artifacts included worksheets of eChem activities, models built by eChem, and webpages designed for final products. During interviews, target students were asked to predict a chemical compound’s polarity and solubility, provide explanations for their predictions, represent an organic compound in various ways, manipulate molecular models mentally, and make translation between various representations.

Data analysis

The pre- and post-tests, including multiple choice and short answer questions, evaluated students’ conceptual understanding of chemical representations before and after using eChem. Process videos provided details about how target students used this visualizing tool and were coded by an analysis scheme. This scheme included students’ actions of using eChem (e.g., constructing models, using visualizing feature, and analyzing properties), their actions with the use of eChem (e.g., reading aloud, writing worksheets, making comments, and discussing), and their interactions with teachers and the researcher (e.g., interventions). The amount of time students stayed in each action of eChem and the frequency students used specific features showed how various features in eChem, such as model rotation and chemical formula, helped students construct models and make translations between representations. We also examined students’ levels of engagement. Engagement is defined by the amount of time students spent on discussions while using eChem. High engagement means that a student dyad spent relatively more time on thoughtful discussions containing back and forth dialogues. These discussions were transcribed and provided rich information for the investigation of how students developed understanding of molecular models.

Semi-structured interviews were conducted after students finished this project to obtain students’ explanations and meanings for representations and investigate students’ understanding. According to students’ responses, their conceptual understanding were coded as correct/accurate, partial, and incorrect, and their ability of translation were coded as high, adequate, and low. Artifacts demonstrated students’ learning progress over time. They were used to triangulate the findings of process videos and interview transcripts. For example, models and information presented on webpages were used to examine whether they were coherent with students’ responses to interview questions and whether students’ preferences of using a particular type of model on webpages influenced their ability to translate representations. Curriculum materials, classroom videos, and field notes of classroom observation offered evidence to examine assertions generated from other data resources. For example, students' preference of using a specific model may be influenced by the frequency of this type of model used in the class. Students' interpretation of chemical representations in interviews may be shaped by explanations that teachers provided in the class. Additionally, because process videos did not record students' physical activities, facial expressions and body languages, the data from classroom video recordings were used to complement and triangulate the findings of process video analysis.

Cases were created for each pair of focus students, and cross-case analysis was used for determining the commonalties, differences, and difficulties of translating representations and model construction. To draw conclusions, the data analysis involved generating assertions by searching the data corpus, establishing an evidentiary warrant for the assertions and verifying assertions by confirming and disconfirming evidence.

Results

A paired two-sample *t*-test for means shows statistically significant difference between means of pre- and post-tests (t=13.9, $p<.001$). Moreover, the effect size indicates that the average score on the post-test was more than 2.5 standard deviations greater than the average score on the pre-test (effect size=2.68). Although this study did not include a control group and the learning effects by instructions and the use of technological tool were inseparable, these results show that after this 6-week project, students acquired content knowledge at the macro and microscopic levels and were able to translate various chemical representations.

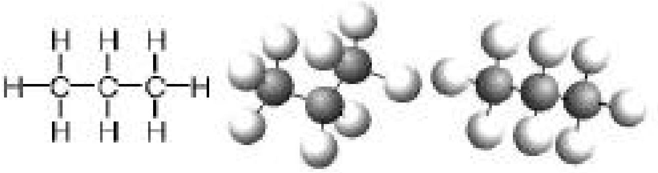
A number of themes related to students' engagement, conceptual understanding, and use of eChem emerged from the qualitative data analysis and synthesis.

Theme 1: The higher the engagement with the use of eChem, the deeper the conceptual understanding of chemical representations.

In this study, engagement is defined by the amount of time students spent on discussions while using eChem. Based on the frequency of discussions and the amount of time spent on thoughtful discussions, target student dyads are categorized as high (3 dyads), adequate (4 dyads), and low (2 dyads) engagement groups. Analysis of interviews shows that high engagement students demonstrated more accurate and correct conceptual understanding in terms of properties, structures, and underlying concepts. They were able to represent an organic molecule in various ways, describe visual differences between these representations based on the underlying concepts such as bonding theory, identify isomers by viewing two-dimensional models, and apply underlying concepts to justify their predictions or explanations about representations.

Process videos provide data for possible explanations of how students' engagement was correlated to their conceptual understanding. When students were highly engaged in constructing, visualizing, and/or analyzing molecular models, their discussions involved the conceptual aspect of representations through which students made these representations meaningful. For example, during eChem activity one, students were asked to construct alkanes, but one pair of high students was unsure which bond arrangement of carbon was appropriate for a propane model. They clicked on the sp^2 hybrid orbital, and then found that this bond arrangement made the number of hydrogen atoms less than their prediction. It made them wonder whether the model they created was propane or not. Through building a propane model on eChem, these two students constructed (and redefined) their meanings of hydrocarbons, alkanes, and chemical bonds. During the class instruction, they acknowledged that hydrocarbon compounds were composed by carbon and hydrogen atoms. However, they did not realize how complicated chemical bonding of a hydrocarbon compound could be until they constructed this propane model. Bond arrangements provided by eChem encouraged them to consider that different bond arrangements influenced the number of hydrogen atoms attached on carbon atoms, even though the total number of bonds a carbon atom has is always the same. They also learned what counted as an alkane, which was a type of hydrocarbons with only single bonds as the compound they created, propane. Moreover, they applied their knowledge of organic chemistry and integrated the knowledge of bonding and hydrocarbons to accomplish the task. Thus, high engagement students' discussions involved the conceptual aspect of representations, such as bonding and the definition of alkanes, and that the bond arrangement feature on eChem potentially promotes students to explore various bond arrangements, search for patterns, and make chemistry bonding meaningful.

In addition to the conceptual aspect of representations, process videos show that for these high engagement students, the process of making sense of 3D models involved the visual aspect of representations. During the project, structural formulas and other 2D representations were introduced to students before they used eChem. These hand-drawing or printed 2D structures became the symbol system (Salmon, 1979) that students were familiar with. The first challenge for students to make sense of 3D view of molecules was to decode the information of bond angles and geometry of molecules that were not represented by 2D structures (Fig. 3(A)). Analysis of process videos shows that all high engagement students consciously rotated a 3D propane model from Fig. 3(B) to Fig. 3(C), because (C) looked similar to a linear 2D structural formula on paper. Through this model rotation process, the 3D model were more meaningful for students, since it shared similar visual features of the 2D one, such as relative location of hydrogen and carbon atoms and a linear carbon chain. Thus, identifying visual similarity between representations is critical for students to make sense of a novel representation.



(A) (B) (C)

Figure 3. A 2D structural formula and 3D models of propane

Theme 2: Both physical and computational models served as a thinking vehicle for students to manipulate mentally.

During final interviews, in response to structural differences between two structural formulas, the majority of students formed and manipulated a model mentally. As students described, their mental images were built on physical or computational models shown or used in class activities. For example, in response to an interview question, identifying whether two structural formulas were representing the same molecule, Steve said,

> Those are different. Now I'm picturing the examples like Mark [the teacher] did with the little models [physical models] with the springs. You can't turn it like here the chlorine and CH3. They are on the opposite sides you know. Here is on the same side. You can't just turn it, because the double bond doesn't work that way; you can't just twist it.

Another student, Jerry, thought both eChem and physical models helped him visualize 3D models. Being asked about which models he manipulated mentally to answer questions in terms of 3D models, Jerry said,

> Both actually. I like eChem; you know, you are able to rotate them. This thing [physical model] of course you know, it's in you hands, when eChem is only on the computer.

These two segments illustrated that physical and computational models were carriers of students' mental images, although these two types of models have different symbol systems (Salomon, 1979). In additional, students noticed the limitations and advantages of these two types of models that manipulating physical models provided concrete feelings of models and that eChem models were easily rotated, created, and modified.

Theme 3: The process of visualization involved retrieving relevant information and activating verbal and non-verbal connections in individual cognition.

To translate a chemical formula to a structural formula, some of the target students formed a mental image prior to drawing a 2D model. During the interview, in order to translate a chemical formula, C_5H_{10}, to a structural formula, one student compared this formula with the general formula of alkanes, and then transformed this formula to a mental image of what C_5H_{10} may look like.

> (The interviewer shows them a chemical formula, C_5H_{10}, and asks the students translate it to a structural formula.)
> S1: is it cyclopentane? (Looking at his partner, S2.)
> S2: what?
> S1: It's like a circle. (Using figures to make a circle.) It's not pentane, because it's C five, H twelve.

> Interviewer: How do you know that?
> S2: Because the formula for it, is it 2n+2?
> S1: If you get carbons, two hydrogens attach each carbon, except the ends. (Using one hand to show a linear carbon chain, and moving the other hand to locate where hydrogen atoms are around this chain.)
> S1: I am thinking cyclopentane, because there aren't extra two.

The process video showed that during eChem activity I, these two students generated the general formula of alkanes by themselves based on various alkane models they built on eChem. The excerpt above indicated that they developed a conceptual linkage between formulas and structures, which included the information of symbols, structures, and mental images. They compared the unfamiliar representation, C_5H_{10}, to their prior knowledge about the reasonable number of hydrogen atoms and what an alkane should look like. They then retrieved the relevant information to make formula-to-model translation. By elaborating the idea of general formula and externalizing their mental models through verbal and non-verbal interactions with the interviewer, these students demonstrated the process of visualizing a chemical formula.

Furthermore, this excerpt reveals the interweaving nature of visualization and conceptual understanding in chemistry which could be illustrated by Paivio's dual coding theory (Clark & Paivio, 1991; Paivio, 1986). This theory explains how verbal and non-verbal representations associated with each other in individual cognition. During eChem activities, student 1 and 2 constructed a conceptual connection (connection 1) between the chemical definition of alkanes and its general formula, a visual connection (connection 2) between structural formulas and correspondent mental images, and referential connections (connection 3) between this general formula and their mental images. When they encountered the question of translating C_5H_{10} to a structural formula, all these connections were activated. Examples of connection 1 are the following comments by S1 and S2 respectively: "It's not pentane, because it's C five, H twelve." and "Because the formula for it, is it 2n+2?" S1 externalized Connection 2 through his body language and speaking out that "If you get carbons, two hydrogens attach each carbon, except the ends." As Mayer and Anderson (1992) indicated, problem-solving transfers required both representational and referential connections. To determine that C_5H_{10} could be cyclopentane, S1 needed to activate the referential link to identify that C_5H_{10} did not fit the general formula and then triggered other possible models to solve this problem. Therefore, the process of visualizing C_5H_{10} involved making or activating the connections between verbal and non-verbal representations.

Theme 4: While models serve as a vehicle for students to construct mental images, different types of 3D models were not used interchangeably for these students.

Both physical and computational models served as a thinking vehicle for students to manipulate mentally. In response to interview questions that probed understanding of structural differences between two structural formulas, the majority of target students formed and manipulated 3D models mentally. Yet, different types of 3D models were not used interchangeably for these students. Among three types of 3D models, all target dyads chose ball-and-stick models as their 3D representations on final products. During interviews, when students were asked to identify functional groups and compare structural differences, students spent relatively less time to come up with answers if they were allowed to view the ball-and-stick models. Although the process videos showed that space-filling models were the most visually attractive to students, students did not prefer to use them to identify functional groups because bond orders were invisible in this type of models. Therefore, while wire-frame models may be too abstract by showing only carbon chains and space-filling models do not demonstrate bond orders directly, the ball and stick models were the most concrete ones for students because they convey the visible information of atoms and bond orders.

Feature analysis

As discussed previously, the rotation feature in eChem helped students made sense of 3D representations. This feature also assisted students to construct models. Process videos showed that the majority of students frequently used model rotation to make empty bonding sites visible. The chemical formula displayed on the *Construct* page assisted students to identify empty bonding sites and translate a structural formula into a 3-D model. After using eChem for one week, some target students explored features which were not mentioned by worksheets. For instance, they frequently used "Extras" and "Fragment" as shortcuts for model construction. The "Extras" feature allowed them to fill out all hydrogen atoms by one click, and "Fragment" provided long carbon chains and a benzene ring. These two features were both designed to simply the complexity of model construction. However, when encountering technical problems, none of students read the Help message—a feature designed to scaffold the learning process.

Discussions and Conclusion

Computational models and chemistry learning

Recent research has suggested that using computational and physical models could promote chemistry learning (e.g., Copolo & Hounshell, 1995). The present study provides empirical data to support the learning benefits of using models. The result of pre- and post-tests of this study shows the positive learning effect of using a visualization tool in a project-based classroom. The visualization tool, eChem, promoted students to develop conceptual understanding of chemical representations through constructing models and viewing multiple representations. eChem specially improved students' ability of translating 3D models to 2D representations and this ability is important for students to understand the concepts of isomers and polarity. While eChem assisted students to develop understanding of chemical representations, this study does not attempt to conclude that either the computational model or the concrete model is the best for chemistry learning. Rather, through analysis of interviews and process videos, this study suggests that both types of models should be provided by class instruction because different students have different preferences.

Additionally, this study reveals how students made meanings of various representations and constructed visual and conceptual connections. Two eChem features are crucial for these processes. First, while bond arrangements limit students' capability to construct unstable compounds (e.g., CO and ozone), they promote students to apply chemical concepts they have learned to choose appropriate bondings. The action of selecting bond arrangement strengthens and/or builds students' conceptual linkage among bonding, structures, and molecules. Second, model rotation feature provided by eChem assists students in making visual connections between 2D and 3D models. For students who had visual experience of 2D structural formulas, a 2D-like model (Fig. 3(C)) was easily to be decoded, whereas visualizing Fig. 3(B) needs to deal with the bond angles, representations of atoms, and the bent carbon chains. This feature lowers the cognitive burden of visualizing 3D models, externalizes the mental rotation process, and supports students to make translations between 2D and 3D models. While the empirical studies have shown a moderate correlation between spatial ability and learning achievement in chemistry (Carter, LaRussa, & Bodner, 1987; Pribyl, & Bodner, 1987), through externalizing the metal rotation process, eChem might enable students with low spatial abilities to rotate and visualize chemical compounds.

Therefore, eChem has capabilities for students to develop and practice representational skills. Given the notion of developing representation competence through chemistry instruction (Kozma & Russell, 1997), eChem provides a range of opportunities for students to identify structural differences with various representations, make translation among them, and select appropriate representations to solve problems. Implemented with learning activities, eChem extends students' understanding of atoms, chemical bonds, and molecules.

Students' preferences of molecular models

In Harrison and Treagust's study (1996) of students' mental models of atoms and molecules, students had a strong preference to select the space-filling molecular model as a better representation of a molecule. Similar to their finding, two target students used both ball-and-stick and space-filling models to represent their toxin on their webpage and called the latter model as "a more realistic depiction." However, without showing bond orders, the space-filling model was not the most visualizable model for students to identify functional groups and make translations during interviews. Thus, although the ball-and-stick models do not demonstrate appropriate atom sizes and electron cloud surrounding atoms, using them to provide a concrete experience of chemical bonds, atoms, and molecule is necessary for high school students. After students develop basic understanding of bonding, teachers could provide various 3D models and guide group discussions of how different models convey different information of bonding, atom size, and electron. Through class discussions, students would be able to realize limitations and benefits of using different types of representations and learn to appropriately use different models to solve problems as chemists do.

The role of visual connections in chemistry learning

While the literature emphasizes the conceptual aspect of visualization in chemistry, the results of the study reveal that constructing visual connections between representations is as important as making conceptual connections for chemistry learning. Analysis of process videos show that reconstruction of a conceptual connection could be initiated by a visual conflict. To make sense of novel representations, students need visual similarities between their prior visual experience and the new one. While the studies of novice and expert indicate that novices tend to rely on the surface features of representations to categorize representations and solve problems (Chi & Feltovich, 1981; Kozma & Russell, 1997), this study further implies that chemistry learning could be built on novices' sensibility of the surface features. Surface differences in representations may not be a learning barrier; rather, through the discussion and negotiation of meanings with peers, these surface or visual features could assist students to reconstruct their understanding, visualize abstract representations, and make translations. Teachers could encourage students to ask questions related to visual differences of representations and discuss how these differences may or may not share different meanings in chemistry.

Dual coding theory and visualization in chemistry

This study applies Paivio's dual coding theory to illustrate how the target students visualized a chemical formula. Visualization is a process involving the conceptual-verbal and visual-nonverbal connections within individual cognition, which could be also supported by the analysis of interview transcripts. The analysis indicates that students who could translate 3D to 2D models may or may not be able to translate chemical formula to structural formula. The later translation process may involve visual, conceptual, and referential connections, while the 3D-to-2D translation could be achieved by solely comparing visual features of these models. Namely, visualization and difficult translations need the establishment of referential connections between verbal and non-verbal systems (Mayer & Anderson, 1992).

Summary

This study was designed to investigate following research questions: 1) Are students able to translate between two-dimensional and three-dimensional representations? If so, in what ways does eChem help students to translate between representations in chemistry? 2) What patterns do students demonstrate while translating chemical representations and constructing models by using eChem? How do these patters reveal students' development of conceptual understanding of chemical representations? The test results show that by using the visualizing tool, eChem, for six weeks, the majority of eleventh graders were able to translate between two-dimensional and three-dimensional representations. Their abilities of identifying functional groups, describing structural differences, and translating representations significantly improved.

Analysis of the video recordings of target students reveals that several features in eChem, such as model rotation and chemical formula, helped students construct models and translate representations. Some students frequently engaged in thoughtful discussions and compared structural differences between various representations. These discussions involved both visual and conceptual aspects of representations, which in turn deepened their understandings of representations. Compared with the space-filling and wire-frame models, the ball-and-stick model was the most concrete one for these high school students. The results suggest that both physical and computational models can serve as a thinking vehicle for students to manipulate mentally. These mental images helped students to translate representations and identified structural differences of organic compounds.

For the future investigation, we would like to explore how chemical representations are taught and learned through class interactions, whether and/or how the use of eChem shapes students' conceptions of atoms and molecules, and whether and/or how the use of eChem engages class members to make connections among three levels (macroscopic, microscopic, and symbolic) of chemistry through class interactions.

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