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A MODEL OF MOLECULAR VISUALIZATION

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Abstract: We argue that molecular visualization is a process that includes constructing a mental model. Current qualitative research has shown that participants working on a mental molecular visualization/rotation task invoke components of a mental model. Four of the components are static representations: referents, relations, results, and rules/syntax. The fifth component is dynamic: operation. Two examples of operation are visualization and rotation. Participants used the constructed mental models as mental tools to complete the task. This conceptualization of mental model construction constitutes a theory of learning.

ANTECEDENTS

Research from several domains suggests that molecular visualization is a process of mental modeling that uses both representations and operations. To support this claim we draw from both the previous literature and results of our recent research. More than 50 years ago, the social psychologist Morton Deutsch (1951) wrote, “Men think with models.” Similar conclusions were reached by Ludwig Wittgenstein (1961), who suggested that people picture (or visualize) facts to themselves and that a model is a picture (or visualization) of reality. In this chapter, we use the terms visualization and representation to refer to specific kinds of mental activity. We will presume that visualization is a mental operation and that representation is the object and result of that operation.

Johnson-Laird (1989) developed the concept of mental modeling as the foundation for model-based reasoning and suggested the basis for a relationship between visualization, as defined above, and mental model construction. Various authors have argued that mental models contain at least one dynamic component that is called an operation (Tuckey & Selveratnam, 1993; Lesh, Hoover, Hole & Kelly, & Post, 2000). We argue that visualization is an operation that produces a one-to-one correspondence between a mental representation and the idea, object or event to which it refers (the so-called referent). Visualization can therefore serve as the dynamic component that supplies the material with which model-based reasoning occurs. This reasoning is a personalized activity, however, because individual reasoners construct their own mental models (Bodner, 1986; von Glassersfeld, 1989). We therefore suggest that reasoning in general can be conceptualized as mental model building but the individual models constructed are idiosyncratic and personal (Kelly, 1955). Current research (Briggs, 2004) supports this conclusion.

METHODOLOGY

A qualitative research methodology allows one to access mental constructs that are difficult or impossible with a quantitative approach (Bodner, 2004). Our chosen methodology was phenomenography (Marton, 1981; Svensson, 1997) because it seeks to answer what we argue is a third-order question. A first-order question might be, “What is the world like?” A second-order question could be, “How do I experience the world?” A third-order question is, “How do I conceptualize my experience of the world?” Our conclusions in this chapter arose from the study of conceptualizations of the experience of mental molecular rotation by undergraduates either taking or preparing to take organic chemistry. In this study, the third-order question being considered was, “How do participants conceptualize and articulate their experience of mental molecular visualization and rotation?”

To develop theory of mental modeling we wanted to study the mental structure and processes involved in visualization and mental model construction. We could do that using the metaphor given by Marton (1981) of “figure” and “ground.” In this metaphor, comprehended content is “figure” and the act of comprehension, is “ground.” This perspective on process versus content enables one to focus on the cognitive activities rather than the content processed by those activities. The objective was to obtain for study the articulations of the conceptualizations of the experience of mental molecular rotation.

In order to generate a data stream of articulations we chose to use the technique of individual interviews that involved a think-aloud protocol (Simon & Ericsson, 1993). Participants worked on tasks in which they were required to mentally rotate a given two-dimensional molecular representation and produce a drawn artifact of the rotated molecule.

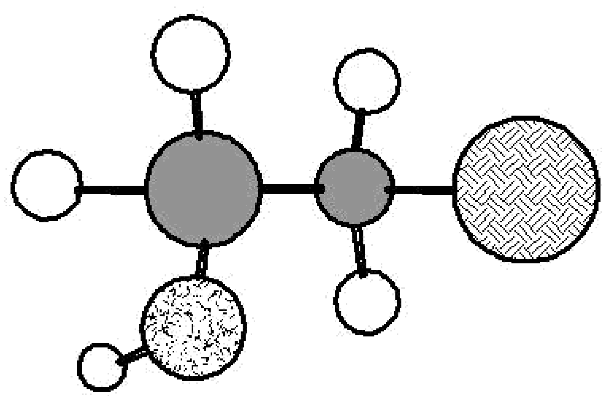

Figure 1: Example of a task molecule given to participants. The grey filled circles represent carbon atoms; the unfilled circles represent hydrogen atoms; the random filled circle represents an oxygen atom; and the weave filled circle represents a halogen atom

While working on each task, the participants were encouraged to verbalize what they were thinking at the moment. The various tasks used in this study were classified in order of increasing difficulty on the basis of three criteria: the number of atoms in the molecule, the extent of branching of the carbon chains, and the degree of rotation about each axis. We presented each task as a color-coded representation filling a 10 cm x 20 cm rectangle. The compounds whose molecular representations were used in this study consisted primarily of carbon and hydrogen atoms, but each compound had at least one oxygen or nitrogen atom as a reference for the rotation instruction.

We recorded each participant’s articulations on both audio and video tape and collected the drawings they produced during their work as an artifact of the interview. After transcribing the interviews, we coded them in the tradition of grounded theory (Strauss & Corbin, 1998). Analysis of the resulting codes allowed us to develop a theory of mental model construction based on the visualization and mental rotation of molecules.

Multiple participants were used to allow us to compare and contrast the articulations and the conceptualizations of the participants in order to, "... understand in a limited number of qualitatively different ways ..." (Walsh, 1993) the answers to the third-order question we asked. The study design was cross-case with thick description. In the following section, we present some of the thick description in the form of interview vignettes as support for claims we make regarding the representations and operations of mental molecular rotation and visualization.

STUDY RESULTS

During the coding of the transcripts, we paid particular attention to articulations that indicated components of a mental model (Lesh, Hoover, Hole & Kelly, & Post, 2000). We felt that evidence of the use of components of mental models by the participants would support a claim for the construction and use of mental models. We found ample evidence of the construction and use of mental models as the following vignettes illustrate. We have arranged this information in accord with the five components of a mental model as described by Lesh, et al. (2000): referent, relation, rules/syntax, operation, and result. Narrative vignettes were chosen from the work of the five participants in this study, who were given the pseudonyms: Oslo, Julia, Chessuana, Pete, and Ryleigh. All of the participants were second-year organic chemistry students at Purdue University.

Referents

Referents are physical objects, labels for objects, and mental representations. The participants acknowledged the use of referents during their work on the tasks. For example, Oslo noted, "So, if I stick with the carbon that we are focusing on ...." In this case, Oslo selected a carbon atom in the task molecule and used it as a reference point for determining the relative positions of other atoms in the rotated molecule. Oslo clearly distinguished one atom from the other atoms in the molecule. Making that distinction is critical to completing the task of visualizing and rotating the molecule. In another task, Ryleigh says, "Since this is the one [atom] that they are physically asking me about, that is the one that I'm going to physically rotate around." In a similar statement, Chessuana responds, "And, I would pick, presumably, this corner [atom] right here." In another task, Oslo offers, "Since the line of sight would be drawn from this carbon to this carbon ..."

Note that each of the participants indicates a specific atom within a molecule. Failure to distinguish atoms in one of tasks molecule would seem to prevent one from visualizing the task molecule. The point is clear in Julia's articulation, after sitting silently for many seconds, "Because I'm having difficulty with this chain here. Like putting that into space." Careful analysis of the transcript to her interview suggested that Julia had chosen a group of atoms but could not visualize them in space because she was not making distinctions between the atoms in this group and therefore could not place them into proper relation in mental space. The failure to distinguish among individual atoms may indicate a defective or missing visualization operation and would prevent a participant from constructing a useful mental model of the task molecule. We therefore argue that one of the components for a model of visualization of molecules is a defined referent.

Relations

The second component of our model of molecular visualization is relation, which involves the spatial relationship between referents. While working on one of the tasks in our study, for example, Ryleigh reported, “And there were two hydrogens off of that carbon, both going to the back of the page, so now they will come to the front just slightly to the left.” In this vignette, Ryleigh focuses on the spatial relation among three atoms. There are three elements of this relation: position in space (109 degrees apart), sequence in bonding (hydrogen-oxygen-hydrogen), and identification of each atom (two hydrogens and one carbon). Ryleigh indicates a significant amount of chemical knowledge in this short statement, including the notion of tetrahedral bond angles, atom valences, and atom electronegativities. Working on another task, Chessuana states, “What I’m trying to do here is I’m trying to take this red oxygen [atom] and then somehow flip this molecule so that these two oxygens are one on top of the other so that I can’t see one oxygen atom.” In this statement, Chessuana identifies two oxygen atoms in the task molecule and thinks aloud about their relation to one another both before and after the rotation. In his interview, Oslo demonstrated the component of relation by referring to a carbon by position in the task molecule, “... then I’m going to move to the carbon on the left side here, that’s with the *t*-butyl group, the number two carbon ...” Several relations are defined in this statement. Oslo identifies a carbon as “number two”, indicating sequential relations between the carbon atoms in the backbone of the molecule. Oslo also identifies a connectivity relation between the central carbon of the *t*-butyl group and the number two carbon atom.

On a different task, Julia commented, “... then this one [atom] appears to be even more farther back, farther away, then somehow this has to connect to the blue (atom) ...” Julia’s comment was based on a relation between two atoms in terms of “behind” or “in front of”. Julia seemed to know specific atoms are related by connectivity in the task molecule, but could not see the relationship in the rotated molecule. She used the word “somehow” to indicate this uncertainty.

Another aspect of the component of relation is between the observer and the observed. Chessuana demonstrated this relation by saying, “I guess when I’m looking at something, I would imagine myself to be at the origin of a three-dimensional axis system.” This aspect of relation is directed from the observer to a virtual observer rather than the relation between the observer and the observed shown in the preceding vignettes. This relation resembles the notion of perspective taking in the work of Piaget and Inhelder (1956). In an interesting comment, Julia combines these two types of relation, “... the vertical orientation is not going to change just by walking around to the other side of it.” The relation of the atoms within the molecule, indicated by the phrase, “the vertical orientation,” is a relation within the molecule. Julia then referred to a mental representation of the task molecule that took a perspective as if looking at the molecule from another side; Julia seems to be thinking from the perspective of a virtual observer, a relation external to the referent molecule.

Rules/syntax

A required component of any mental model is a set of rules and syntax by which to order a mental representation. We define “rule” to be a concept and “syntax” to be the method of implementation of this rule. Thus, the rule and its syntax form a system. Our work suggests that mental imaging is not a random collection of mental “pixels” but rather an ordered visualization operation. This implies that a set of rules and syntax must be operating in order to make sense of the visual input from our eyes. Examples of rules/syntax systems that occurred in our study are given below.

Ryleigh expressed the following while drawing an artifact of a rotated molecule, "And the last methyl group [carbon number five] will just retain its tetrahedral shape [draws the three hydrogen atoms]." Ryleigh indicated an important concept associated with mental model construction: bonds in the task representation must be conserved. This conservation includes the number of bonds, their orientation in space, and the identity of the atoms involved in each bond. This is a sophisticated evolution of visualization because it allows the participant to draw a correct artifact of the rotated molecule. An important form of assessment for the researcher or teacher is available at this point. For years, organic chemists have evaluated the maturity of a student's mental model construction by evaluating the artifacts drawn. Domain acceptable application of the rules/syntax component will produce "correct" artifacts.

While working on another task, Chessuana comments, "This carbon atom is going to come out and its, all of its hydrogens are going to be almost completely in view now [after the rotation]." Chessuana has applied another rule: atoms that are occluded by other atoms still exist and follow the rules of conservation. The task from which this comment was generated happened to have all of the methyl hydrogens visible, but Chessuana comments on their visibility because in other tasks the hydrogen and carbon atoms were sometimes hidden behind other atoms. Chessuana's articulation indicates that the rule/syntax component of conservation still holds true in the case of occluded atoms.

Another example of the rule/syntax component is comparison against a standard to check for reality or correctness. Julia demonstrated this comparison by saying, "Which also means the third [carbon atom] will kind of hide the carbon that is behind it, too, because there is the same, like plane going through all of those [atoms]." Julia constructed a mental model of a plane, applied it to the visualized molecule, and then used that construct to compare how other atoms were occluded. The comparison process seems to imply another rule/syntax component: atoms in a plane all move in the same manner when the plane rotates. This component must be an integral part of the constructed mental model of a plane or the result would not be useful.

Oslo used a rule/syntax component that noted that rotation conserves conformation of bonds. "But if we say it stays in this conformation then I can draw it [in rotated form]." And on another task, Oslo noted, "Oh, because it is all bonded to the carbon [atom] it would have to be just like this [draws the rotated molecule]," which is another application of the rule of conservation of bonds.

Another rule/syntax component is based on perspective. Visualization requires some method of indicating objects close to the viewer and other objects farther away from the viewer. In chemistry we often use atom size, bond foreshortening, or a system of hashes and wedges to indicate spatial orientation. The rule/syntax component might be: atoms closer to the viewer are larger than atoms farther away from the viewer; or, the end of a bond coming toward the viewer is larger than the end of the bond farther away from the viewer. Another version of this component might be: bonds along the axis of sight from the viewer to an object are foreshortened but bonds perpendicular to that axis are not foreshortened. These cues to spatial position are required for a student to draw a correct artifact of a visualized and mentally rotated molecule. Oslo, for example, visualizes a molecule as, "... my idea usually is, I have that chain and then I have bonds going away into the page and out of the page." In this case Oslo used the plane of the task representation as a reference for visualizing the molecule. Oslo used the hash and wedge system to show perspective when drawing the rotated molecule. An example of a deficiency of a perspective rule/syntax component was shown by Ryleigh, "I can't picture the entire molecule because there are too many bond angles ...” This lack of a useful rule prevented him from completing the task of visualizing the molecule.

The rule/syntax component of a visualization model is an important part of the visualizing ability. Without this component, participants were unable to make sense of the task molecule and could not visualize it. We assumed that participants who could visualize and mentally rotate a task molecule had a well-developed system of rules and their associated syntaxes. We drew this conclusion from the participants’ articulations of their conceptualizations of the experience of molecular visualization.

Operation

The foregoing components are static in nature, but the component “operation” is a dynamic entity. We define an operation as the process of transforming a representation from one form to another. This might occur, for example, when a two-dimensional task representation printed on paper is transformed into a mental representation. We have called this operation “visualization” and called the product of the operation a “representation.” Another form of this component would involve the transformation of a mental representation by an operation such as rotation to produce a new mental representation. An important operation in our study was the transformation of a mental representation of the rotated molecule to a two-dimensional artifact drawing. Our work suggests that operations are mental activities and components of mental models as the following vignettes show.

Pete demonstrated on operation that involved transformation of a mental representation to a drawn artifact when he commented, “It’s just getting it out onto the paper, drawing it on the paper.” Julia talked about the operation of visualizing by using a plane, “Let’s see, I’m kind of like trying to split it [Julia uses here hands to indicate a plane] and seeing what would be on what side.” Chessuana referred to the operation of rotation by saying, “And I would know that this green [atom] would be rotated the farthest from the end and come all the way around and two carbons, I suppose these are, in the middle, would just stay in the middle.”

Note the dynamic nature of these examples. There seems to be a fundamental difference between this component and the others we have investigated. Operation is different from the other components in its ability to transform a referent. Each of the other components involve more or less static representations, but operation involves transformation of a referent. We have noticed that this static-dynamic relation plays a role in the structure and processes of mental model construction.

Our participants invented operations to mitigate deficiencies in visualization abilities. Ryleigh illustrates this process by saying, “It’s large enough and complex enough that it’s too hard to do that [visualize the whole molecule]. So, I come up with sort of a formula, and know if this is the front and this direction [left or right], and I rotate it 180 degrees that way, then it would be in the back now, and so, then all I have [to do] is kind of plug and chug with each bond.” Ryleigh breaks the operation of molecular rotation into an operation on each atom in the molecule. This invention worked fairly well on small molecules but broke down on larger ones. Another problem with operation was shown by Pete in this vignette, “My problem right now is actually, when I rotate anything, instead of rotating the molecule as a whole, I’m just sort of twisting it around a bond.” Pete realized that a deficiency existed but did not invent a correct operation to replace rotation. Oslo invented a way of assisting the rotation operation by chunking or combining atoms into groups. This was shown by, “...

it's pretty easy of you have a grasp on how these methyl groups are oriented, it's pretty easy to visualize a tripod and to flip the whole thing around." If the components known as referents, relations, rules/syntax, and operations are correctly constructed then a participant could construct and use mental models to obtain results.

Results

The component "result" is an important part of model-based reasoning because it is the product of operating on a referent. We use the term "result" to convey both mental and physical products. A mental example would involve visualization producing a mental representation from a conceptualization or a physical object. That is, visualization as an operation produces a transformed representation: a result. A physical product would occur when the operation of transformation, for example, makes a mental representation into a physical artifact

An example of the component known as result that was found in our study is rotational congruence: an operation on one element of a set will yield the same consequence as the same operation on another element of the set during the mental process of rotating a molecule. Julia demonstrated this when she talked about visualizing a rotated molecule, "... you can't see the ones behind these two methyl groups, because they are going to be hidden just the same as this one ..." On another task, Julia said, "... these two carbons and these four hydrogens would all appear to be, like, in the same plane ... And I'm looking to see if that appears to be the same thing on this side [of the molecule]...." Julia applies visualization to representations from two different media, a mental representation of the task molecule and the drawn artifact. Chessuana visualized in the same manner. Comparing the task representation to the drawn artifact of a rotated molecule, Chessuana comments, "So I know that up here, I have this red oxygen atom, and that looks to me like these are actually kind of going down a little bit, both this oxygen and this other hydrogen." Chessuana confirmed that the result of the task, the drawn artifact of the rotated molecule, was correct.

In each case, the participants operated on a task molecule and produced a result, an artifact of a rotated molecule. Once a participant produced a result, they could use it as evidence of successful completion of the task, to compare the result to the initial representation of the task to determine correctness, and to learn the conformation of the rotated task molecule. The production of a result seems to be sufficient justification for the exercise of mental model construction. The benefit of building mental models outweighs the costs of using mental energy because we learn from our interactions with the world. This learning then frees us from repetitive problem solving or model building.

In the foregoing paragraphs, we have shown the five components of a mental model. Four of those components are static representations: referents, relations, rules/syntax, and results. The component operation is dynamic. Warrants for the evidence presented in support of our claims come from the work of two researchers, Richard Lesh (Lesh, Hoover, Hole, Kelly, & Post, 2000) and Robbie Case (Case, Okamoto, Stephenson & Bleiker, 1996).

WARRANTS

In *Principles for Developing Thought-Revealing Activities for Students and Teachers in Handbook of Research Design in Mathematics and Science Education*, Lesh, et. al, (2000) discuss mental models and their components. We have made minor changes in some of the terms to allow this work to fit research outside the realm of mathematics. The relationship between the components of a mental model can be stated as follows. An operation on a set of referents produces a result. The referents and results (which can, themselves, become referents) are connected by relations and rules. The concept of a mental model is useful and fruitful. Used as a perspective to analyze our study results, we found that participants use mental models to visualize molecules.

The results of our study of molecular rotation raise several questions, including: “What is the consequence of the dichotomy of static and dynamic components of a mental model of molecular visualization?” And, “How do participants determine the reality and correctness of their visualization results?” Possible answers to these questions can be found by combining the work of Lesh, et al (2000) with the work of Robbie Case, et al, (1996).

In Chapter VIII, Summary and Conclusions in *The Role of Central Conceptual Structures in the Development of Children’s Thought*, Case, et. al, (1996) describe a set of structures and processes that account for children’s thought. The hypothesized structures differentiate between central conceptual structures and an executive control structure. We have found these structures to be useful ways of conceptualizing mental model construction. We have come to understand the central conceptual structures as the repository of mental operations that are at the core of mental model construction. We conceptualize the executive control structure as a distinct kind of mental model. The central conceptual structure contains mental operations that one uses to construct short-term mental models as required by reasoning in progress. This type of mental model is fleeting and constructed as needed in the intimate problem solving of reasoning.

The executive control structure is different in both duration and content. We argue that this mental structure is a long-term mental component and contains representations of our lifetime experiences. An example is the lesson we learned as young children that the top of a stove can be very hot. We do not have to relearn this lesson because we securely hold it in memory and can access it to warn us of new surfaces that might be hot. Without such a place in memory as the executive control structure, we would have to repeatedly relearn that surfaces can be hot. The executive control structure is a valuable asset because it frees the mind to concentrate on new and important problems instead of the “... buzzing, blooming confusion...” James (1911) we experience as infants. Our minds are freed from repetitious learning, giving us more processing power to apply to new experiences. The executive control structure functions as a standard by which we construe the world. A manner of conceptualizing this mental control structure is as a worldview. The participants in our study continually checked their work to determine if it was correct and used the executive control structure as the standard for comparison.

The work of Lesh, et. al (2000), and Case, et. al (1996), along with our work indicates that the components of mental models, the central conceptual structure, and the executive control structure form a mental system that is the basis for reasoning and learning. This insight has led us to explanations of several diverse fields of study in the domain of science education.

INSIGHTS

The process of visualization seems to precede the operation of rotation in a task of mental molecular rotation. From the moment one gives the participant the instructions for a task, the participant must visualize referents in order to begin a sequence of mental model construction. The task starts with visualizing words and sentences and turning those symbols into meaningful mental models. Then the participant must visualize the task molecule and transform it into a mental representation. We assume that there is significant processing between the eyes and the brain but will not address that in this chapter. Visualization is a dual media operation: it acts upon physical objects in the world around us and acts on mental objects. When told a technical fact we sometimes say, “Oh, I see it now!” This is not just slang but a semiotic response due to the way we conceptualize the action of the operation visualization.

Improper visualization may cause flawed representation and lead to incorrect results. This is an important lesson to teachers. We must be very careful of the manner and precision with which we scaffold our students as they construct their mental models of domain-accepted concepts. A flawed mental model can have an impact on reasoning beyond what one might expect.

The mind has error correction schemes for visualization that we hypothesize arise from the executive control structure. By having a standard by which to compare what one is visualizing, one can make sense of the object of visualization. This can work against us, however. If one builds an incorrect mental model and it becomes the standard by which one compares new mental models, results at variance with domain-accepted concepts may occur. Each of us has experienced the situation in which an optical illusion has tricked us into interpreting a drawing or picture incorrectly. Once we are shown or recognize on our own the correct interpretation, we can usually force ourselves to see the drawing correctly. The same situation with a flawed mental model, however, can cause the holder to reject what the senses are telling them and accept incorrect results, which has happened repeatedly in the history of science. It is for these reasons that teachers must probe for and demand correct construction of mental models of scientific principles.

IMPLICATIONS

The concept of mental modeling and model-based reasoning explains some examples of learning by providing structure and processes. Research into thought processes support the use, by participants, of the components of a mental model. We have found that participants use their constructed mental models as mental tools to navigate a solution path through a task. When a similar task is given several weeks later, the participants recall the former mental model and use it. We hypothesize that the recall consists of reconstructing the mental model when needed. In this sense, mental model building is a process of learning. The components of a mental model have to be constructed before the model is useful for reasoning. As domain- specific concepts become more complex, the model can be reconstructed using new referents, relations, and operations. The construction of the components and the use of mental models is controlled by maturation (Case, et. al,1996). As a result, younger children do not build models as complex as older children and adults, which limits the concepts that students can learn at a given level of maturation.

Learning is a sequential process. Learners must construct basic models before they can construct complex models. In chemistry, for example, students must construct a model of particulate matter in order to construct a more complex model of gas pressure or dissolution. The construction of a mental model of particulate matter requires models of an individual unit, identity, property, and interaction. It takes time to construct mental models and one can often partially construct the models concurrently. This process of interactive mental model construction constitutes our experience as we try to construe the world around us. Some models that are used frequently or successfully in different contexts become part of our executive control structure and are then available for error correction, comparison, and decision making. Use of the executive control structure allows one to modify behavior based on experience and constitutes a definition of learning.

In some ways, misconceptions and conceptual change theory can be thought of in terms of changes to constructed mental models. As infants, we begin to construct mental models of the world around us; for example the cooing of a mother's voice, the discomfort of being wet, and the motion of objects in front of us. Without training in model building, we build the model as best we can and sometimes the relations and rules are not correct. We might label these incorrect models as misconceptions. Changing the misconception is not an easy task, as secondary teachers will attest. We hypothesize that conceptual change is the process of constructing a new, fruitful model to replace (or coexist) with an incorrect one. It may be possible to change mental models but it seems more likely that one builds a new mental model that competes with the old model for usefulness. The model one uses the most or is fruitful in more situations is reinforced and is more likely to be used next time a similar context develops. As warrant, we offer the example of chemical equilibrium. Students with a well developed model of the particulate nature of matter seem to be able to grasp the dynamic nature of chemical equilibrium better than students who do not have such a model or have a model that is not as well developed. As students see chemical equilibrium in action, solve problems involving equilibrium, and reflect on the concept of equilibrium, they build new models with components that make the model useful. This is evidence that students construct mental models as needed to reason about a concept or problem.

In summary, we would like to argue that models and modeling provides a fruitful perspective on learning. In the study of molecular visualization and rotation described, in part, in this chapter, we have found evidence for the construction and use of mental models by the participants in this study.

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