Computerized Molecular Modeling as a Collaborative Learning Environment

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Abstract: Interpretation of symbols, as well as understanding the particulate nature of matter and spatial structures are essential skills students need for solving problems in organic chemistry. However, model perception and understanding the spatial structure of organic molecules has been a source of difficulty for many chemistry students. A computerized molecular modeling (CMM)-based collaborative learning environment has been shown to be an effective means to overcome certain learning difficulties in chemistry.

This research investigated the effect of using different types of models while teaching organic chemistry on student understanding of new concepts and the spatial structure of new molecules, as well as preference of a particular model type. We employed a teaching method that combines physical (plastic) and virtual (computerized) three-dimensional molecular models in both collaborative and individual learning setting on 276 students from nine high schools in Israel.

Research tools included a designated learning unit, software and database for computerized molecular modeling, and pre-and post-course questionnaires on organic compounds and models.

Experimental group students understood the model concept better and were more capable of applying transformation from one-dimensional to two- or three-dimensional molecular representations and vice versa. Based on these results, we recommend incorporating both virtual and physical models in chemistry teaching/learning as a means to foster spatial understanding of molecular structure.

Introduction

Science can be thought of as an attempt to model nature in order to understand and explain phenomena. A model can be viewed as an intermediary between the abstractions of theory and the concrete actions of experiment. Models have a target — the actual thing they are trying to represent, and a source — the idea or object from which the representation is derived (Hardwicke, 1995). They therefore help making predictions, guide inquiry, summarize data, justify outcomes and facilitate communication (Gilbert & Boulter, 1998).

Brief History of the Development of Molecular Models

The history of models (Walton, 1968; Petersen, 1970; Ramsay, 1981; Hardwicke, 1995; Clark, 1997) can be traced back to Plato (482-347 BC), who conceived of the four "elements" — soil, water, air and fire. Nothing much happened in terms of model development until in 1808 Dalton published the *New System of Chemical Philosophy* — the first substantial discourse on atomic theory. At the same year Malus discovered polarized light. Wollaston related it to tetrahedron, but noted that *"It is perhaps too much to hope that the geometrical arrangement of primary particles will ever be perfectly known"*.

In 1811 Dalton had a set of models of atoms and simple diatomic molecules constructed to help illustrate his ideas. In 1815 Biot observed several organic compounds that enable light polarization and realized that the rotation of light was due to a property of the individual molecule. In 1848 Pasteur found that crystals can be separated into two types, and in solution they rotated the plane of polarized light equally, but in opposite directions. This discovery could not be explained at that time due to lack of a proper model. The next indication of actual model construction was by Kekule in 1867, who proposed the tetrahedral structure of carbon bonds. In 1874 Van't Hoff used models — tetrahedra joined at the apex, sides or faces to describe the optical isomers of tartaric acid, which raised widespread objection.

Sachse was one of the few chemists who around 1890 used molecules to make predictions, and predicted the 'boat' and 'chair' forms of cyclohexane. During 1900-1920 the use of ball-and-stick models became more widespread. In 1934 Stuart developed space-filling models that gave precise indications of the van der Waals radii of the atoms in a molecule. These were preferred over the earlier type, and opened the 'golden age' of molecular models. In 1947 Pitzer computed the energy barrier to carbon-carbon bond in butane. Later, Pitzer and Hazel, who won Nobel Prize in chemistry, demonstrated the axial and equatorial chair form of cyclohexane ring. Space filling models were considered an indispensable tool for organic chemists during the next 30 years and enabled the prediction of structural conformations, strereochemistry, reactivity and physical properties. Most notable was the double helix structure of DNA proposed by Watson and Creek in 1953, who later won Nobel Prize in chemistry.

Models in Science and Science Education

Modeling and simulation are used in research and education to describe, explain and explore phenomena, processes and abstract ideas. Scientists, engineers and science educators use models to concretize, simplify and clarify abstract concepts, as well as to develop and explain theories, phenomena and rules. A model is considered useful if it is simpler than the natural object that it represents. An important value of models in science and science education is their contribution to visualization of complex ideas, processes and systems. A virtue of a good model is that it stimulates its creators and viewers to pose questions that take us beyond the original phenomenon to formulate hypotheses that can be examined experimentally (Toulmin, 1953; Bagdonis & Salisbury, 1994). Experimentation, however, is rarely presented as a way of developing, interpreting or evaluating explanatory models for the investigated phenomenon (Tamir, 1989). Ben-Zvi and Genut (1998) recommended to teach high school students about interconnections of history and philosophy of science on one hand and the usefulness and limitations of scientific models, such as the Periodic Table, on the other hand.

Gilbert and Boulter (1998) distinguish between target systems, mental models, expressed models, consensus models and teaching models. Other researchers underscored the need for models as enablers of students' mental transformation from two-dimensional to three-dimensional representations (Baker & Talley, 1974; Elliot & Hauptman, 1981; Barak & Dori, 1999).

One of the problems that arises while using concrete models is that insufficient emphasis is placed on the fact that models are theory-based simulations of reality. The theory of molecular structure is a kind of intellectual model (Hammond, Osteryoung, Crawford & Gray, 1972). Harrison and Treagust (1996) claimed that the use of term "model" is a source of considerable semantic variation for science students and teachers. Models are often oversimplified and therefore cannot tell humans all they may wish to know about the real physical system that is being modeled.

Teachers and students should, therefore, be made aware of the fact that models, employed in a variety of research, study and design contexts, are not complete representations of the realities they are supposed to represent (Osborne & Gilbert, 1980).

Applied to chemistry, physical ball and stick models derived from polystyrene spheres and plastic straws are not merely enlargements of the molecules they are intended to represent. These are analogue models that are used to explain new and abstract concepts. Some of the properties are similar to aspects of the target they are representing. For example, the relative diameter of the spheres represents the size of the different atoms. Other aspects, however, are not reflected in the model. For example, in a ball-and-stick model type, all sticks (straws) are of equal length, while "real" molecular bond lengths are not. Other analog models focus on different properties of the molecule, thereby creating multiple ways of representing the same molecule. Teachers frequently use just one type of model, limiting students' experience with models and causing their model perceptions to be partially or completely inadequate.

Computerized Molecular Modeling

The use of concrete molecular models (made of plastic, wood and/or metal) to illustrate phenomena in chemistry teaching has been widespread for a relatively long time (Peterson, 1970). The choice of model type has an impact on the image students create concerning the ways in which particles are shaped and how they function in the "real" world from a scientific viewpoint.

Simulating different model types quickly and efficiently is achieved in a computerized environment, of which theoretical chemists, experimentalists and educators are taking advantage (Wilson 1997). Information technology helps relieving present-day researchers and students from the laborious task of data collection and enables them to engage in creative thinking and problem solving. Nakhleh and Krajcik (1994) investigated how different levels of information presented by various technologies affect secondary students' understanding of acid, base and pH concepts. They found that students using microcomputer-based laboratories exhibited a positive shift in their concept map scores, indicating greater differentiation and integration of their knowledge.

The development of computerized molecular modeling (CMM) made traditional models less favorable in the late 1960's. Not only are computers capable of drawing and manipulating molecules in three dimensions. They are also powerful tools for predicting molecular spatial structure through energy minimization calculations based on quantum mechanics. These capabilities have opened the way for advanced research in chemistry, resulting, among other things, winning Nobel Prize in chemistry (1998).

Among the advantages of using information technology in science education are the options of providing for individual learning, simulation, graphics, and the demonstration of models of the micro and macro world (Dori, 1995; Dori & Barnea, 1997**;** Dori & Hameiri, 1998; Krajcik, Simmons & Lunetta, 1988; Krieger, 1996; Lazarowitz & Huppert, 1993). Computer aided instruction enables students to solve a variety of problems while carrying out their own research at their own pace (Dori & Barnea, 1993; Dori 1995). The use of computerized models places more emphasis on the creation of mental models by students and their use to make prediction (Gilbert & Boulter, 1998).

Students need more experience with models as intellectual tools that provide contrasting conceptual views of phenomena, and more discussion of the roles of models in the service of scientific inquiry (Gabel & Sherwood, 1980; Grosslight, Unger, Jay & Smith, 1991). Raghavan & Glaser (1995) recommend that science educators become less concerned with the presentation of facts and concentrate on showing the centrality of models in research and education. However, most educators use a limited number of static models, and do not emphasize the way in which models are created, their essential role in science learning, or their advantages and limitations (Gilbert, 1997; Bagdonis & Salisbury, 1994). Williamson and Abraham (1995) studied the effect of computer animations on college student mental models of chemical phenomena. Animations were used in two treatment situations: as a supplement in large group lectures and as both the lecture supplement and an assigned individual activity. Both treatments increased the students' understanding. They attributed the improvement to the superior formation of dynamic mental models of chemical processes that were made possible by the computer animation.

Research Objective and Setting

Our research objective was to investigate the effect of using various types of models in a collaborative learning environment while teaching/learning organic chemistry. We studied the effects of these variables on student understanding of new concepts and the spatial structure of new molecules, as well as their preference of a particular model type.

We employed a teaching method that combines physical (plastic) and virtual (computerized) three-dimensional molecular models. The combination of physical and virtual model types was designed to benefit from advantages of each type while its disadvantages are compensated for by the complementary type.

Physical models of atoms and molecules are tangible and "real" — they can be touched and manipulated in actual three dimensions. They are, however, limited in quantity, variety of colors and sizes, and are not amenable to any computational operations. Virtual, computer-based models, on the other hand, are only visible as two- or three-dimensional, but they are mere projections of images on the computer screen. Yet, since they are virtual, they are available in unlimited quantities, colors, radii, and model types e.g., stereo line, ball-and-stick, and space filling (Barnea & Dori, 1996). Perhaps more importantly, they can be operated on by complex mathematical functions to calculate their expected 3-D shape by means of energy minimization. Considering the advantages and disadvantages of real vs. virtual models, it was our conjecture that students can benefit from using one alongside the other.

The research population consisted of 276 students from nine high schools in Israel. The experimental group consisted of 154 students who studied according to the innovative method. The control group consisted of 122 students who studied in a traditional method. Control group teachers used models only rarely, and only for demonstration. The research tools included a designated learning unit, software and database for computerized molecular modeling, and pre-and post-course questionnaires on organic compounds and models.

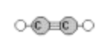
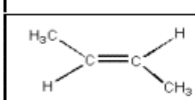
Isomers	Model type	Nomenclature	Molecular formula	The model
				
			C_2H_6O	
				
	Orbit Model			

Figure 1. An example of a problem from the post-organic compound questionnaire

The learning materials were aimed at encouraging students to use different types of models for building spatial structures of organic molecules.

Figure 1 is an example of a problem from the post-organic compound questionnaire that tested the ability to perform bi-directional transformations between one- and two- or three-dimensional representations.

Research Plan

A survey among science and chemistry teachers was first conducted to find what teaching methods teachers use, their opinions regarding the value of using models and actual use of models in the classroom. We considered findings of this survey while developing learning materials for the main research. A pilot study was then conducted to validate the research questionnaires and the learning materials. During the main research, students investigated the molecules' three-dimensional structure, conducted learning tasks and engaged in building and drawing physical and virtual models. The Object Process Diagram (Dori, D., 1995; Dori & Dori, 1996) in Figure 2 describes the structure of the learning materials for both collaborative and individualized learning modes.

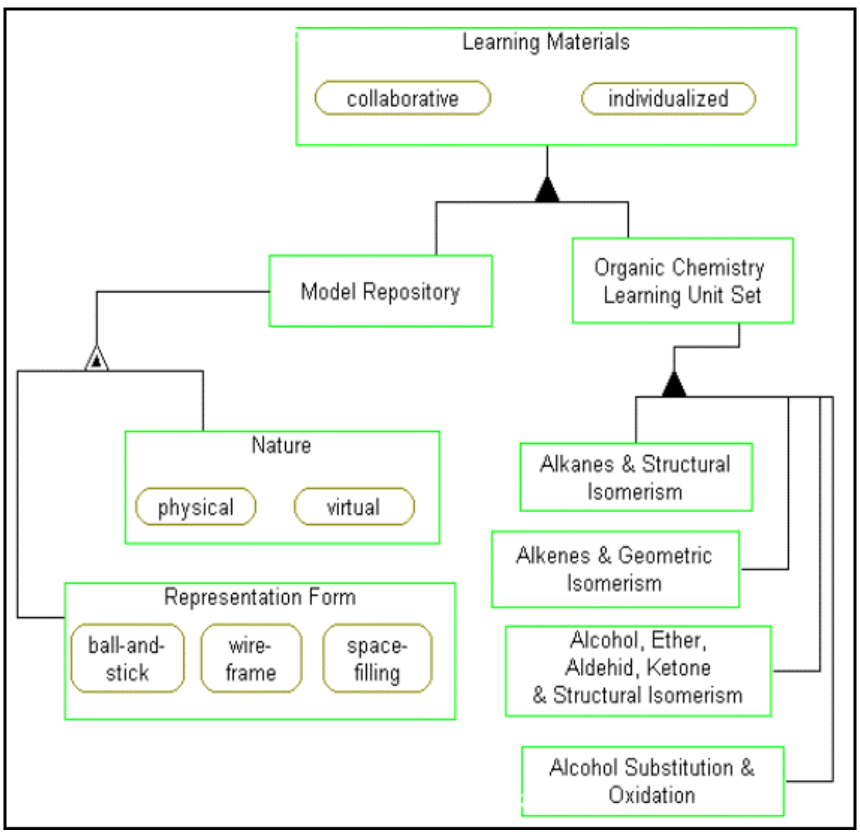


Figure 2. The learning materials and their attributes

The pilot and the main research are described in Figure 3. The expert group, which consisted of science teaching researchers, graduate students, and expert teachers, was the agent for the learning materials developing process. The science teaching researchers team developed and improved the evaluation tool-set, which consisted of questionnaires, observations and interviews. The pre-and post questionnaires related to the model concept and organic compounds understanding. The resulting learning materials comprised a model repository and an organic chemistry learning unit set. The pilot study, carried out by the graduate students and expert teachers, used the model repository and evaluation tool set to improve the learning unit. In the main research we investigated the effect of the computerized molecular modeling and physical models environment on the experimental high school students' learning.

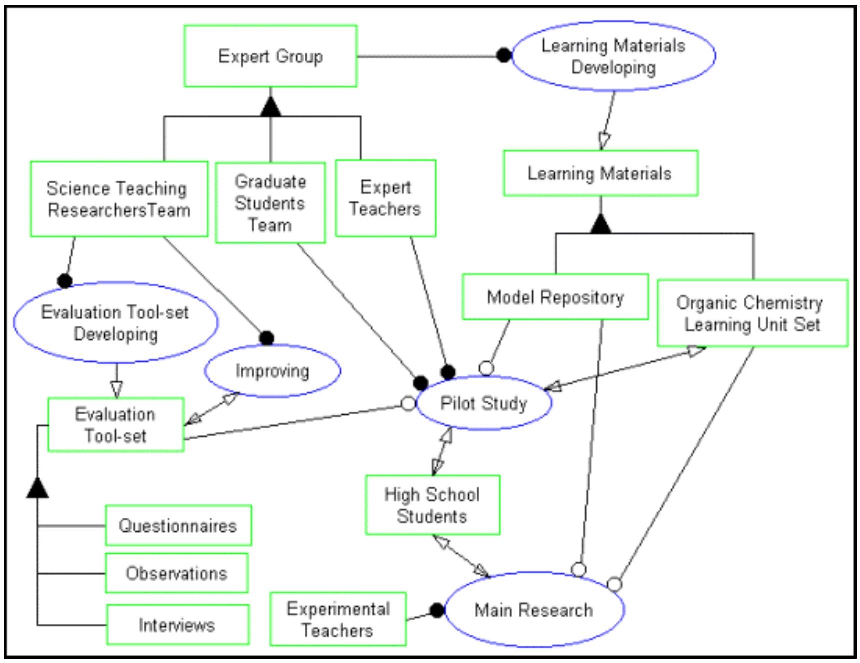


Figure 3. Object-Process Diagram (OPD) describing the research

Research Results

The results of the survey done among 20 science teachers and 31 chemistry teachers regarding the use of models are presented in Table 1. We investigated the types of models and the topics in which the various models were incorporated.

As Table 1 shows, the most prevalent model is ball-and-stick, and the two most popular topics in which models are used are simple molecules and organic compounds. Most teachers indicated that they use models in cooperative learning (32%) and demonstrations (51%). Only a minority (17%) indicated the use of models in individualized learning and attributed it to budgetary constraints. Consequently we decided to supply additional model kits and the CMM software for the purpose of the experiment.

Table 1. The use of models in various chemistry topics

Topic / **Model type**	Simple molecules	Organic compounds	Lattice: ionic, metal or molecular	Macro molecules	Particles	N_1*
Ball and stick	14	8	3	-	1	**26**
Space filling	5	9	2	1	-	17
Orbit (skeletal)	6	7	3	1	-	**17**
Wooden for lattices	2	-	8	2	1	**13**
Magnets	-	-	-	-	3	**3**
Dough	2	3	-	1	-	**6**
Paper	-	-	-	2	1	**3**
CMM	2	3	-	-	1	**6**
N_2**	**31**	**30**	**16**	**7**	**7**	**91**

*Number of positive responses to the use of models for a particular model type.

**Number of positive responses to the use of models for a particular topic.

Pilot Study Findings

The feedback from the pilot study included teachers' and students' open responses to the learning unit and to the learning environment. Overall, the responses were positive and included four categories: interest and understanding, autonomous learners, 2- and 3-D models, and learning skills.

Student negative responses included the need for more explanations, increased competition among students, and the requirement to draw models. Points for improvement teachers indicated related to "waste of precious learning time" and the excessive length of the post-organic compounds questionnaire. We took these remarks into account while improving the learning unit and the post-test for the main research.

Main Research Results

Students' answers to the pre-model and pre-organic compounds questionnaires were analyzed and scores were summarized. The average score of the experimental group was compared to the average score of the control group and analyzed for randomness of the class effect in this research. The results showed that in the pre-model questionnaire there was no significant class effect while in the pre-organic compounds questionnaire a significant class effect was found ($Z=2.01$, $p=0.0450$). Significant differences between experimental and control students were found neither in the pre-model questionnaire nor in the pre-organic compounds questionnaire. Nonetheless, the pre-questionnaires served as covariant in the Mixed Model Procedure (Littell, Milliken, Stroup & Wolfinger, 1996) for analyzing the post-questionnaires results. The new teaching method was determined as the fixed effect and the class was determined as the random effect.

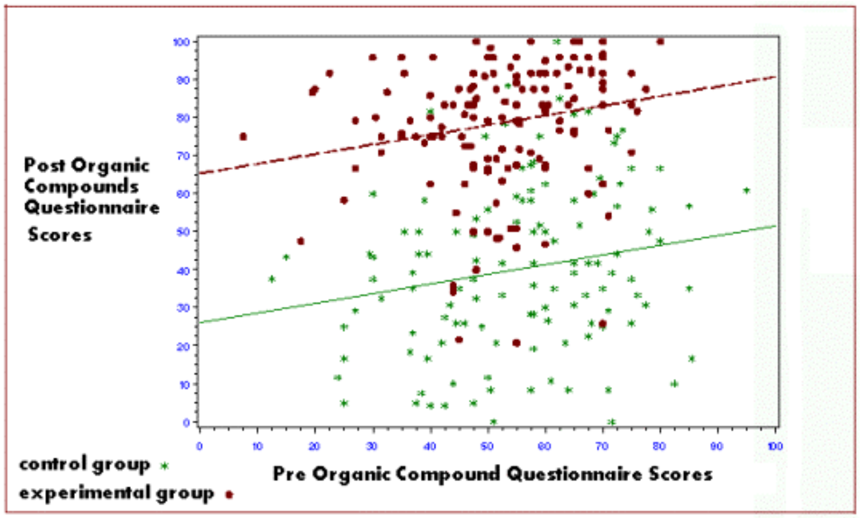


Figure 4. Regression lines for organic compounds questionnaire

Figure 4, which presents the regression lines for the organic compounds questionnaire, shows a steady gap between the experimental and control group scores. The gap is in favor of the experimental group and is statistically significant ($t = —17.12$, $p < 0.00001$). A similar effect was found for the model questionnaire. To examine the effect of the learning method on students' ability to perform bi-directional transformations between one- and two- or three-dimensional representations, we analyzed the results of the problem from the post-organic compound questionnaire, shown in Figure 1. The two significant factors, which were found to explain the students' scores of this problem, were the pre-questionnaire score ($F = 171.3$, $p = 0.001$) and the research group ($F = 6.8$, $p = 0.01$).

Experimental group students understood the model concept better and were more capable of defining and implementing isomerism and functional group concepts than their control group counterparts. They were also more capable of applying transformation from one-dimensional to two- or three-dimensional molecular representations and vice versa. When required to explain their choices, most of the experimental group students used mainly sketches of ball-and-stick models and some space-filling models. Most students of the control group did not provide any explanation (although required to do so) and those who did, used mainly 2-D wireframe model that resembles their teacher's chalk and board structural formulae.

Summary

Interpretation of symbols, as well as understanding the particulate nature of matter and spatial structures are essential skills students need for solving problems in organic chemistry. However, model perception and understanding the spatial structure of organic molecules has been a source of difficulty for many chemistry students. A computerized molecular modeling (CMM)-based collaborative learning environment has been shown to be an effective means to overcome certain learning difficulties in chemistry.

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