VIRTUAL AND PHYSICAL MOLECULAR MODELING:

FOSTERING MODEL PERCEPTION AND SPATIAL UNDERSTANDING

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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 chemistry. However, model perception and understanding the spatial structure of organic molecules has been a source of difficulty for many chemistry students.

The research objective was to investigate the effect of using virtual and physical models while teaching organic chemistry on student understanding of new concepts, the spatial structure of new molecules, and preference of a particular model type. The research involved a new teaching method that combines two types of three-dimensional molecular models: physical (plastic) and virtual (computerized). The research population included 276 students from nine high schools in Haifa and the northern part of Israel.

Experimental students gained a better understanding of the model concept and were more capable of defining and implementing new concepts, such as isomerism and functional group. They were better capable of mentally traversing across four understanding levels in chemistry: symbol, macroscopic, microscopic and process. Experimental group students were more capable of applying transformation from two-dimensional representations of molecules, provided by either a symbolic or a structural formula, to three-dimensional representations – a drawing of a model, and vice versa. Based on the research findings, we recommend incorporating both virtual and physical models in chemistry teaching/learning as a means to foster model perception and spatial understanding of molecular structure.

Keywords: modeling/models, visualization, organic chemistry, spatial understanding

THEORETICAL BACKGROUND

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 help making predictions, guide inquiry, summarize data, justify outcomes and facilitate communication (Gilbert & Boulter, 1998). 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. 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 (Bagdonis & Salisbury, 1994; Hardwicke, 1995; Raghavan, & Glaser, 1995; Toulmin, 1953). Researchers underscored the need for models as enablers of students' mental transformation from two-dimensional to three-dimensional representations (Baker & Talley, 1974; Dori & Barak, 1999; Eliot & Hauptman, 1981).
The use of concrete molecular models to illustrate phenomena in chemistry teaching has been widespread for a relatively long time (Peterson, 1970). 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 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. Theoretical chemists, experimentalists and educators are taking advantage of computerized environment in order to stimulate different model types quickly and efficiently (Kozma, 1999; Wilson 1997). 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 innovative 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 & Barnea, 1997; Krajcik, Simmons & Lunetta, 1988; Gabel & Sherwood, 1980). Williamson and Abraham (1995) studied the effect of computer animations on college student mental models of chemical phenomena. The researchers argued that the animations helped students understand the subject matter better while improving their ability to construct dynamic mental models of chemical processes.

Chemistry students find it hard to connect among the molecular formula, the geometric structure and the molecule characteristics (Gabel & Bunce, 1994; Johnstone, 1991). Understanding the particulate nature of matter, interpretation of symbols and visualizing spatial structures of molecules are essential skills students need for solving problems in chemistry in general and in organic chemistry in particular (Barnea & Dori, 1999; Dori, 1995; Dori & Hameiri, 1998; Barak & Dori, 1999). Many students experience difficulties in understanding topics related to organic compounds (Ryles, 1990; Schmidt, 1992; Shani & Singerman, 1982; Simpson, 1983). These difficulties are explained by the need of students to learn many concepts, theories and processes (Brook 1988; Simpson, 1983).

**RESEARCH OBJECTIVE, SETTINGS AND POPULATION**

A survey was conducted among 20 science teachers and 31 chemistry teachers regarding the use of models. We investigated the types of models and the topics in which the various models were incorporated in chemistry or science courses. The most prevalent model was found to be ball-and-stick, and the two most popular topics in which models were used were 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 active learning. The teachers who used models in demonstration mode only, attributed this to budgetary and time constraints, such as the cost of plastic models or the cost of a computerized molecular modeling software package and the need to “cover” many topics in a short period of time. Consequently, we decided to supply additional model kits and the CMM software for the purpose of the experiment.

Our research objective was to investigate the effect of using physical types and virtual models on student understanding of new concepts and the spatial structure of molecules, their preference of a particular model type and modes of explanation. The teaching method combined 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 the complementary type compensates for its disadvantages.

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, radiuses, 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.

**RESEARCH PLAN**

A pilot study was 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 1 describes the structure of the learning materials for both collaborative and individualized learning modes.

![Figure 1. The learning materials and their attributes](image)

The pilot and the main research are described in Figure 2. The expert group, which consisted of science teaching researchers, graduate students, and expert teachers, was the agent for the learning materials developing process. The resulting learning materials comprised a model repository and an organic chemistry learning unit set (see examples in Appendices 1 and 2).
The science teaching researchers team developed and improved the evaluation tool-set, which consisted of pre-and post questionnaires related to the model concept and organic compounds understanding. There were two versions of the model questionnaire. Students who received version a of the model questionnaire in the pre-test, received version b in the post-test and vice versa. A statistical analysis revealed no difference between the two model questionnaire versions. The pre-course organic compound questionnaire included questions about bonding and molecular structure (students’ prior-knowledge). The post-course organic compound questionnaire included questions that required explaining concepts studied in the topic organic chemistry, such as isomerism, functional groups, substitution, understanding structures of compounds and drawings of models.

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. Figures 3 and 4 represent assignments from the learning unit. The assignment described in Figure 3 appears in the Alkanes topic while the assignment in Figure 4 is a sample of an assignment from the last part of the learning unit.

The following problem deals with four representation modes of different molecules.

- Identify each molecule and write down its name.
- Build a virtual and physical model of each molecule.

**Figure 3. A sample of an assignment from the Alkanes topic in the learning unit**
The following problem contains a chain reaction and a pool of drawn models.

- Match the letters A, B, C and D with the model that represents the appropriate compound.
- Write the name of each compound.
- Identify which molecules are isomers.
- Predict whether molecule D can react with K_2Cr_2O_7 / H_3O^+. If your answer is “yes”, write the product’s molecular formula, if your answer is “no”, explain why.

All the models that appear in the learning unit were drawn by the Desktop Molecular Modeling (DTMM) software that students used.

In the main research we investigated the effect of using computerized molecular modeling and physical models environment on the experimental high school students’ learning and compared their performance to that of their peer students in the control group.

**Research Results**

Students’ answers to the pre-model and pre-organic compound questionnaires were analyzed and scores were summarized. The average score of the experimental group was compared to the average score of the control group. No significant differences were found between experimental and control students in the pre-model questionnaire and in the pre-organic compound questionnaire. Nonetheless, the pre-course questionnaires served as covariate in the ANCOVA model for analyzing the post-questionnaires results. The students’ scores in the pre-course questionnaires also served for categorizing students from each research group into three academic levels: high, intermediate and low. In the ANCOVA model we also took into account the possible dependence between scores of students in the same class, (intraclass correlation). Students in the same class usually tend to be more similar in their scores than students in different classes. This dependence violates the assumptions of the classical ANCOVA regression model, which assumes independence among all observations. The MIXED procedure of SAS (Littell, Milliken, Stroup & Wolfinger, 1996) enables to test the significance of the intraclass correlation and to account for it in the test which compares the experimental vs. the control group. The results showed that in the pre-model questionnaire there was no significant intraclass correlation, while in the pre-organic compound questionnaire a significant correlation was found (p=0.0450).
The Organic Compound Questionnaire

The organic compound questionnaire was designed to determine whether and to what extent the new teaching method improves concept understanding and bi-directional transformations. We also examined students' preference for a particular model type.

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

<table>
<thead>
<tr>
<th>Isomers</th>
<th>Model type</th>
<th>Nomenclature</th>
<th>Molecular formula</th>
<th>The model</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₃C</td>
<td>Orbit Model</td>
<td>..........</td>
<td>C₂H₆O</td>
<td>..........</td>
</tr>
</tbody>
</table>

Table 1 is an example of a problem from the post-organic compound questionnaire that tested the ability to perform bi-directional transformations between one- (molecular formula) and two- (structural formula, ball-and-stick model drawing) or three-dimensional (space-filling model drawing) representations.

Figure 5. Regression lines for organic compound questionnaire
Figure 5, which presents the regression lines for the organic compound 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 ($t = -17.12$, $p < 0.00001$). To examine the effect of the learning method on students' ability to carry out bi-directional transformations between one- and two- or three-dimensional representations, we performed an in-depth analysis of individual problems that were presented to the students in the post-organic compound questionnaire. The two significant factors, which were found to explain the higher performance of the experimental student scores for these problems were the pre-course questionnaire score ($F = 171.3$, $p = 0.001$) and the research group ($F = 6.8$, $p = 0.01$).

Another research aspect we addressed was the different modes students used to explain their answers in the question that dealt with identifying models and isomers in the organic compound questionnaire. Three modes of explanations were defined: textual, graphic and a combination of the two. The assumption was that the experimental group students, who learned by the new teaching method, used physical and virtual models and drew them, would provide explanations that are expressed graphically or in a combination of text and graphics. Indeed, Table 2 shows a significant difference between the research groups regarding their modes of explanation. The Wilcoxon 2-sample test (Mann Whitney) shows a significant difference between the research groups for all three academic levels combined. This difference implies that students in the experimental group were capable of providing more explanations in all three modes (textual, graphic and the combination of both) than students in the control group.

Table 2. Comparison of research groups regarding modes of explanation

<table>
<thead>
<tr>
<th>Modes of Explanation</th>
<th>Mann Whitney</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Z</td>
</tr>
<tr>
<td>Textual</td>
<td>3.78</td>
</tr>
<tr>
<td>Graphic</td>
<td>7.07</td>
</tr>
<tr>
<td>Combination</td>
<td>2.42</td>
</tr>
</tbody>
</table>

To characterize the differences within each research group individually, frequencies of the three modes of explanation were calculated. Figures 6 and 7 show the different modes of explanation by academic levels among experimental group students and control group students, respectively.

Figure 6. Characterizing different modes of explanation by student academic levels among experimental group students

The results clearly show that the gap, which had existed in the pre-course organic questionnaire, between high and low academic students was almost closed for the experimental students. The corresponding gap for the control group, however, was still noticeable. In particular, over 60% of both low and intermediate academic level students could still not provide any explanation whatsoever. In the experimental group only less than 20% of the corresponding academic levels did not provide any explanation.

![Figure 7. Characterizing different modes of explanation by student academic levels among control group students](image)

To investigate students understanding and implementation of the three representation modes, we looked into their ability to carry out bi-directional transformations between two/three dimensions and one dimension, and the ability to identify/draw isomers of a given molecule. Table 3 summarizes the results. Experimental group students scored higher than their control group counterparts, demonstrating the contribution of incorporating virtual and physical molecular models into organic chemistry.

### Table 3. Understanding and applying representation modes by research groups

<table>
<thead>
<tr>
<th>Modes of Representation</th>
<th>DF (degrees of freedom)</th>
<th>t</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wireframe</td>
<td>134</td>
<td>4.59</td>
<td>0.0001</td>
</tr>
<tr>
<td>Ball-and-stick</td>
<td>106</td>
<td>6.14</td>
<td>0.0001</td>
</tr>
<tr>
<td>Space-filling</td>
<td>111</td>
<td>7.79</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

To gain insight into the specific types of model students preferred to use in their explanations, we analyzed the question that dealt with bi-directional transformations between one- and two-dimensional representations. Figures 8 and 9 show the distribution of preferred model representation for the experimental and control student groups, respectively. The results for each group are presented separately for each one of the three academic levels – low, intermediate and high.
As Figure 8 shows, the experimental students favored the ball-and-stick, followed by wireframe model type. Only few used the space-filling model or did not respond to this question at all. About half of the control students, on the other hand, chose not to respond to this question. Most of those who did respond used wireframe, as Figure 9 shows.

A possible explanation to this difference in model type preference can be attributed to the similarity of the wireframe representation to the structural formulae, which the conservative teaching style employs. The results were found to be statistically significant by the Mann-Whitney test for each one of the three representation modes (p < 0.0001).

The Model Questionnaire

The model questionnaire was designed to find out how the new teaching method contributes to the understanding and applying of the model concept. The average score of the experimental group was compared to the average score of the control group. The statistical analysis of the results shows a high significant difference between the research groups. The experimental group students defined the model concept better and they were able to identify model characteristics and their functions better (F=38.23, p=0.0001).

A pattern similar to the regression lines for the organic compound questionnaire (Figure 6) was obtained also for the model questionnaire. It too shows a constant gap between the experimental students scores (regression line intercept = 46.8) and control students scores (intercept = 29.0). The gap is in favor of the experimental group and is statistically significant (t = -6.18, p < 0.0001).

We compared the research groups regarding their ability to apply transformations among four chemistry understanding levels: symbol, macro, micro and process. Figure 10 shows that the average score of the experimental group students at all three academic levels was higher than that of the corresponding academic levels of the control group students. It also shows that students, who were classified in the pre

model questionnaire as having intermediate or low academic level, succeeded in narrowing the gap between them and the high achievers by scoring high in the post questionnaire.

![Figure 10. Post model questionnaire average score for transformation ability among four chemistry understanding levels](image)

The differences between the two research groups regarding transformation ability among four chemistry understanding levels were significant (p< 0.01).

**DISCUSSION AND SUMMARY**

Understanding the particulate nature of matter and spatial structures, as well as interpretation of symbols are essential skills students need for solving problems in organic chemistry. Students at all levels find chemistry one of their more difficult courses (Gabel, 1998). Several review studies (Gabel & Bunce, 1994; Krajcik, 1991; Stavy, 1995) suggested that science educators and teachers need to promote conceptual understanding and non-algorithmic problem solving methods. Other scholars argued that chemistry educators need to examine teaching strategies that help students gain better scientific concept understanding accepted by the scientific community (Treagust, Duit & Fraser, 1996).

Model perception and understanding the spatial structure of organic molecules has been a source of difficulty for many chemistry students (Dori, 1995; Dori & Barak, 1999). To alleviate these difficulties we have presented an innovative teaching/learning approach. Until recently, scientists and researchers almost exclusively used computerized molecular modeling. In this study we introduced both virtual and physical models in an organic chemistry curriculum and studied their effect on enhancing meaningful learning in chemistry. 276 students from nine high schools in Israel participated in this study. Research tools included a designated learning unit, computerized molecular modeling software and database, and pre- and post-course questionnaires on organic compounds and models.

The learning unit included theoretical background on organic compounds and inquiry–based learning tasks that involve building and drawing 3D models. We found that the inquiry–based learning tasks encouraged understanding of organic compounds and provided students with tools for explaining their answers. Experimental group students were more capable of defining and implementing isomerism and functional group concepts than their control group counterparts. 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. Whereas most control group students did not provide any explanation for their answers, most experimental group students explained their answers correctly. An interesting finding was that experimental low academic level students expressed their explanation graphically. We can argue that students’ gradual discovery of the molecules’ 3D structure through model building and drawing enhanced their learning abilities. It enabled them to provide correct answers and explain their answers textually, graphically or the
combination of both. Experimental group students understood the model concept better and were more capable of applying transformation from one-dimensional (molecular formula) to two-dimensional (structural formula or ball-and-stick model drawing) or three-dimensional (space-filling model drawing) molecular representations and from 2D or 3D back to the one-dimensional representation.

The significant improvement in experimental students’ understanding can be attributed to their increased exposure to virtual and physical models and the active learning these students were engaged in. In 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. For example, the relative diameter of the spheres represents the size of the different atoms, or all the sticks (straws) are of equal length, while "real" molecular bond lengths are not. Space-filling models focus on different properties of the molecule. While the experimental students were using various model types they were able to mentally construct multiple representation modes for the same molecule. Teachers in the control group used just one type of physical model, limiting students' experience with models and causing their model perceptions to be partially or completely inadequate. These results are in accord with the finding of Barnea & Dori (2000).

Based on these results, we recommend incorporating a combination of virtual and physical models in chemistry teaching/learning as a means to foster meaningful learning and spatial understanding of molecular structure.

REFERENCES


