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RESEARCH REPORT
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COMPUTERIZED MOLECULAR MODELING - THE NEW TECHNOLOGY FOR ENHANCING MODEL PERCEPTION AMONG CHEMISTRY EDUCATORS AND LEARNERS

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ABSTRACT: Insufficient emphasis is put in science teaching on the fact that models are simulations of reality based on a certain theory and that molecules are not miniatures of the models that represent them. We investigated how chemistry teachers and high school students who enrolled in a special program perceive the nature and functions of models by using a model perception questionnaire. In the research 34 pre- and in-service teachers attended a 14 hours workshop on models and their model perception was investigated with the model questionnaire. This questionnaire was also administered to two groups of high-school chemistry students – experimental and control – which studied chemical bonding and structure. The teachers of the experimental group participated in the training and emphasized the model concept via using various models including computerized molecular modeling, whereas the control group teachers taught the topic in the traditional way, without the aid of computer and without emphasizing the model concept. Overall, the in-service training on models has improved several aspects of the teachers' model perception in both stages. This finding is confirmed by the significant difference found between the experimental and control groups of the high school students. Students' results indicate the effectiveness of the treatment on students' conceptualizing the meanings of models, especially in the domain of chemistry. [*Chem. Educ. Res. Pract. Eur.*: 2000, *1*, 109-120]

KEY WORDS: *computerized molecular modeling; model perception; high-school chemistry; in-service training*

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INTRODUCTION

Modeling and simulation are used in research and education to describe, explain and explore phenomena, processes and abstract ideas. A great virtue of a good model is that by suggesting further questions it takes us beyond the phenomenon we began with to formulate hypotheses that can be experimentally examined (Toulmin, 1953; Bagdonis & Salisbury, 1994). It is recommended that science educators should become less concerned with the presentation of facts and concentrate on showing the centrality of models in research and education (Raghavan &

Glaser, 1995). 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; Oversby, 1995). According to Gilbert Boulter (1998) models are differentiated between target systems, mental models, expressed models, consensus models and teaching models. One way of performing a simulation with different model types quickly and efficiently is by a computerized environment. The use of computers in science and technology teaching has various advantages. Among these are the options of providing for individual learning, simulation, graphics, and the demonstration of models of the micro and macro world (Dori, 1995; Dori & Hameiri, 1998; Lazarowitz & Huppert, 1993). Computers enable students to solve a variety of problems while carrying out their own research at their own pace.

The use of molecular models to enable visualization of complex ideas, processes and systems in chemistry teaching has been widespread for a long time (Peterson, 1970). The choice of the type of model has an impact on the mental image that the student creates. One problem that arises while using models is that insufficient emphasis is placed on the fact that models are theory-based simulations of reality. Applied to chemistry, 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 analog 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, but other aspects are not reflected in the model; all straws are equal, while bond length 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. 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).

The aim of this study is to investigate how chemistry teachers and students perceive the nature and functions of models. Teachers’ perceptions are important, since if teachers do not have the necessary understanding of the nature and role of models in the development of a discipline, they probably will not be able to incorporate them properly in their teaching (Gilbert, 1991; Barnea & Dori, 1996).

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 and Sherwood, 1980; Grosslight, Unger, Jay and Smith, 1991). Harrison and Treagust (1996) found out that most 8-10 graders prefer models of atoms and molecules that depict these entities as discrete, concrete structures and therefore, prefer space-filling molecular models. To enhance understanding a multiple range of models should be used, as students prefer the use of computerized molecular models instead of the plastic ones (Barnea, 1997; Dori and Barnea, 1997).

RESEARCH GOAL AND POPULATION

The goal of our study was to develop a computer molecular modeling (CMM) learning environment via implementing a constructivist approach in high-school chemistry, and to examine its effect. Teachers' and students' perception of the nature and functions of models were investigated by using a model perception questionnaire.

The research included two populations and was administered in two stages. The first stage included 34 teachers who participated in an in-service training.The second stage was implemented in an urban high school in Israel, involving five heterogeneous classes (N=169) of tenth graders (age 15) who studied chemistry for the first year. The experimental group – three classes (N=97) – worked on the subject of geometric shapes of molecules with the molecular modeling software and a dedicated working booklet. Two other classes, which served as a control group (N=72), studied the subject in the traditional way.

Four teachers were involved in the second stage, two taught the experimental group and two the control group. All the teachers had academic degrees in chemistry and at least 15 years of teaching experience.

RESEARCH METHODOLOGY

The CMM software and working booklet

The software tool used in the study was the "Desktop Molecular Modeler (DTMM)" (Crabbe & Appleyard, 1994 - this package is published by Oxford University Press, Walton St. Oxford OX26DP, UK), a PC-compatible package which enables three- dimensional molecule visualization. Several representation styles – colored lines, space filling, quick filling and ball and stick – are available. The software is controlled through pull-down menus, which are easy to master. The most powerful features of the software are molecular synthesis and energy minimization (Gulinska et al., 1991). The energy minimization routine optimizes the geometry of the newly created molecule by using an algorithm that creates the optimal three-dimensional conformation.

As part of the research we have designed and written a self-study booklet, which fosters a constructivist learning approach of various geometric shapes of molecules (Barnea & Dori, 1999).

Teachers' training – First stage

The pre and in-service teachers (N=34) attended a 14 hour workshop on models and modeling. During the training teachers learned the different meanings of models and experienced various types of models. They discussed in small groups the difference between mental models, expressed models, consensus models and teaching models, and tried to categorize models they use into these classifications.

Teachers spent 6 hours familiarizing with the molecular modeling software. They worked with a database that was especially designed by the researchers for the high-school curriculum. Teachers chose molecules from the data-base, measured their bond length and angles, rotated them and watched them in various styles: bonds only, stereo lines, ball and stick and space filling.

After the information gathering stage, teachers checked whether the geometric shapes they viewed for those molecules, were consistent with their prior knowledge. Where mismatches were found they discussed the advantages and disadvantages of the models, thus getting more acquainted with the abilities and limitations molecular modeling offers as a teaching tool.

Experimental group – Second stage

The teachers of the experimental group participated in the training and emphasized their new insight of the model concept while using various models including computerized molecular modeling. The experimental group—three classes of tenth graders—participated in three computer laboratory sessions of two hours each, and used the database described above. Since the computer laboratory had only ten workstations, students worked in pairs and had the opportunity for interactions and group work. Students chose molecules from the database, measured their bond length and angles, rotated them and watched them in various styles: bonds only, stereo lines, ball and stick and space filling. Students also used stereo view glasses to get a 3D perception of molecules.

After the information gathering stage, students decided what geometric shape those molecules had. Later, they discovered the similar properties of molecules that shared the same structure by building their Lewis formula. These students could identify the graphic representation easily, and this, in turn, helped them decide whether the molecule is polar or non-polar. Sometimes, the teacher used rigid models in order to clarify some misunderstandings, stressing the differences among the various models. Students discussed in group the advantages or disadvantages of each model, enhancing their understanding of models and modeling. During the sessions students were very enthusiastic and concentrated on their work, discussed the results and conclusions with their peers, and called for assistance or approval of the teacher only when they disagreed or could not find a proper answer.

Control group – Second stage

The two teachers of the control group participated in the training too, and were familiar with the computerized molecular modeling package. They chose to teach in the traditional way without the aid of the computer out of their free will, and (possibly) anxiety of computers. The control group—two classes of tenth graders—studied the geometric shapes of molecules in the traditional way in the classroom, and used only one type of plastic models.

Model questionnaire

We examined the perception of the model concept among pre- and in-service chemistry teachers in the first stage of the study. In the second stage of the research we examined model perception among high-school students that were taught by these teachers. The research tool was a questionnaire on models in general and on models in chemical bonding and structure in particular. It is a revised version of the first part of the questionnaire of Barnea et al (1995). In this part, responders were asked to mark and explain if they agree, partially agree or disagree with 16 statements.

The second and the third parts of the questionnaire were developed especially for this research (Barnea, 1996). The second part of the questionnaire related to the use of models in chemistry and contained open questions related to bonding and structure. The third part dealt specifically with models used in chemistry. The responders were asked to specify model type(s) which are used to explain the following examples of visible phenomena.

1. Copper in the solid state conducts electricity.
2. Gaseous chlorine does not dissolve in water, whereas, hydrogen chloride gas dissolves well in water.
3. Solid graphite conducts electricity, while diamond does not.
4. Sodium chloride does not conduct electricity in solid state, but it conducts electricity in an aqueous solution.

As a result of the first stage of the study analysis (in-service training) the following change was incorporated in third part of the questionnaire. Graphic representations were added to represent models, and responders were asked to write the name of model/s or to describe the chemical phenomena these models represent. When items were given textually, responders were asked to draw the appropriate model which explains this phenomena. Exemplary items of the third part (after modification) are presented in Table 1.

The 16 statements in the first part were divided into four categories by the researchers. Four experts in chemistry education were independently asked to read the questionnaire and

TABLE 1. *Exemplary items from the third part of the model perception questionnaire.*

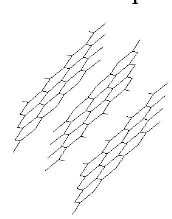
The phenomenon	The model which explains the phenomenon
1.	The model which describes the energy levels of the electron in the atom. Electrons fill these levels in a regular pattern: 2, 8, 18, etc.
2. Solid Copper conducts electricity	
3.	
4. Gaseous chlorine does not dissolve in water	
5.	The structure of C– Graphite. 

TABLE 2. *Categorized items from the first part of the model perception questionnaire.*

Category 1 *Models describe and explain phenomena*	**Category 2** *The model as a mental or a representative structure*	**Category 3** *Ways to create models*	**Category 4** *The model as a tool for research and prediction*
* The only function of models in science is in teaching.	* The terms 'model' and 'theory' are synonymous.	* All models are creations of the human intellect.	* Models are aids that are used to obtain knowledge of nature
* A model always provides a complete description of the object, structure or process in nature that it models.	* Any representation of a structure or of a process is called a model.	* Models exist in nature.	* Models can be used to predict phenomena structures or processes that have not been observed.
* Models play an important role in the explanation of phenomena.	* A scientist has more knowledge of an object, process or structure that is represented by the model.	* A model is formulated using facts obtained by experiment and/or observation.	* Models play an important role in scientific research, in medicine and the drug industry.
* An important function of any model is to describe an object, a process or a structure in nature.	* All models are representations (some are purely visual, some can be touched).	* All models are mental images i.e. exist only in the human mind.	* Models are temporary. With the increase of knowledge a model becomes obsolete or useless and is either adapted or replaced by another model.

divide the statements into categories to check the validity of the decision. The categories thus obtained are the following: models as describing and explaining phenomena; models as mental representations; model generation and models as prediction and research tools. Table 2 represents the 16 questionnaire items divided into the four categories.

RESEARCH RESULTS

The model perception questionnaire was administered to pre- and in-service chemistry teachers, as well as to high-school students. The score consisted of four sub-scores: a score for each part of the questionnaire and a score on the categories in the first part.

- **Part I** is the sum of the scores gained on the 16 statements using the following scale: *completely agree* - 2, *partially agree* - 1, *oppose* - 0. Opposing statements got the opposite score, i.e., *fully agree* got the score 0 whereas *oppose* scored 2. Since each statement/item scores between 0 and 2, the total score ranged between 0 to 32.
- **Category** sums the knowledge of the different categories and ranges from 0 to 4. Each category consists of 4 items. Each item has a maximal score of 2 therefore the score on a category can range from 0 – 8. In order to get a score 1 on a category, one has to receive at

least 5 out of 8 possible points given on a category. If one gets less than 5 points, one's score will be 0 in that category. The sum of these scores results in the Category score. If a responder knows all four categories, his/her score will be 4.

- **Part II** summarizes the second part of the questionnaire, which includes three open questions. In this part the responder has to verbally define a model (item no. 17), give three examples for various models that are used in chemistry (item no. 18), and explain what is the role of models in chemistry (item no. 19). The answers to these statements were categorized into levels. Statements 17 and 18 got scores ranging from 0 to 3 and statement 19 could score from 0 to 4, overall the third score could range from 0 to 10. In this way item 19 gets more weight than the other two, but this question deals with the highest level of understanding. While item 17 requires knowledge, and item 18 is a question of application, item 19 requires analysis of the definitions and examples in order to generalize the role of a model, which is a much heavier task. Some examples for representative answers and their scores are presented in Table 3.
- **Part III**, given to the third part of the model perception questionnaire, relates to eight items. A score of 0 was given to a wrong answer, 1 was given to a partial or verbal explanation, where as 2 was given only if a full explanation was accompanied with a graphical description. The maximum score could thus be 16.

Teachers' results

The teachers' scores on the various parts of the questionnaire are represented in Table 4. 34 pre- and in-service teachers took part in the workshop and answered the questionnaire. From Table 4 we see that even after the intensive training, some of the scores are still not high in the research population. We can relate this result to the difficulties that arise when a clear and unequivocal definition of the model concept has to be formulated. This is a problematic issue, as the model concept is known intuitively but there is usually no definite distinction among model,

TABLE 3. *Exemplary responses and their given score in Part II of the model perception questionnaire.*

Item No.	Student Response	The Score
17. Define a model	* A model is an exact copy of reality	1
	* A model is developed in order to explore a certain phenomenon by overlooking or stressing some aspects	2
	* A model is developed in order to pursue an idea or to perform a research	3
18. Give three examples for various models that are used in chemistry	* Models of the atom, like ball and stick	1
	* Various models of lattices - more than one example	2
	* Models in chemistry which do not deal with the atom structure - more than one	3
19. Explain what is the role of models in Chemistry	* The models support understanding	1
	* A model describes and simplifies phenomena	2
	* A model relates between micro to macro	3
	* A model helps to predict events and phenomena	4

TABLE 4. *Mean scores and standard deviation of the different parts of the model perception questionnaire for the pre- and in-service teachers (N=34).*

Score	Mean	S.D.	Minimum	Maximum	Range
Part I	23.30	2.73	17	29	0-32
Category	2.94	1.12	0	4	0-4
Part II	5.54	1.78	0	10	0-10
Part III	7.67	2.89	2	14	0-16

theory and reality. Moreover, the ways in which models are created are not clear.

In Table 5, the correlation coefficients among the various parts of the questionnaire are represented. We can see high and significant correlation between part I of the questionnaire and the category score, and between part II and the category score. In other words, the category score is in high correlation with both the general part and with the chemical part of the questionnaire.

Analysis of the teachers' responses to the Part II, the open part of the model questionnaire, revealed that most of the participants thought of a model as a way to describe a process or a phenomenon which could not be seen. A distinction between a mental image and a concrete model that can be seen and touched was made. There was agreement among all responders that models help explain and understand phenomena through simplification and visualization.

The examples given for the use of models in chemistry were all in the domain of atomic and molecular structure. Most teachers perceive models as a means to enlarge or reduce the real process or phenomenon, or to illustrate some theory. Only few teachers thought of models as mental images.

TABLE 5. *Correlation's among the different parts of the model perception questionnaire for pre- and in-service teachers (N=34).*

	Part I	Category	Part II	Part III
Part I		0.743 **	0.02 ^{ns}	0.306 ^{ns}
Category			0.380 *	0.118 ^{ns}
Part II				0.05 ^{ns}

^{ns} $p > 0.05$
* $p < 0.05$
** $p < 0.0001$

TABLE 6. *Analysis of variance (ANOVA) of students' mean scores on total score for the model perception questionnaire.*

Source of Variance	SS	df	F	p
Research group	2009.30	1	14.10	0.0002
Gender	455.25	1	3.20	0.076
Interaction*	142.62	1	1.00	0.319

* (Research group * gender)

High school students' results

An overall score for the model questionnaire was calculated, by summing its four components, such that each part had the same contribution to the total score. Analysis of variance, shown in table 6, indicates that there is a significant difference between the research groups. However, no significance was found for gender or interaction between gender and research group factors.

Similar results were obtained when this analysis was done for each part of the questionnaire independently. Significant differences in favor of the experimental group were found regarding Part I, Part III and the score for Category. For Part II however the difference is not significant. The results are presented in Table 7.

A thorough investigation into items 17-19, which compose the second part of the questionnaire, revealed that the experimental group students scored higher on items 17 and 19, but the control group students did better on item 18. The corresponding results for the students as well as the teachers in the second phase are shown in the Figure. In item 18, responders were requested to specify three different types of models, which are in use in chemistry. After the experimental students had experienced intensively the computerized molecular modeling, most of them gave examples from their practice in this area: ball and stick or space filling models, diamond or graphite models, etc.

TABLE 7. *Mean scores, standard deviation and t-test procedures of different parts of the model perception questionnaire by research group.*

Score	Group	N	Mean	S.D.	t	p
Part I	Experimental	86	21.20	3.35	3.41	0.0008
	Control	64	19.22	3.71		
Category	Experimental	86	2.67	1.12	3.62	0.0004
	Control	64	2.00	1.16		
Part II	Experimental	86	3.98	2.18	1.19	0.235
	Control	64	3.55	2.14		
Part III	Experimental	86	3.79	3.08	4.45	0.0001
	Control	64	1.88	2.20		

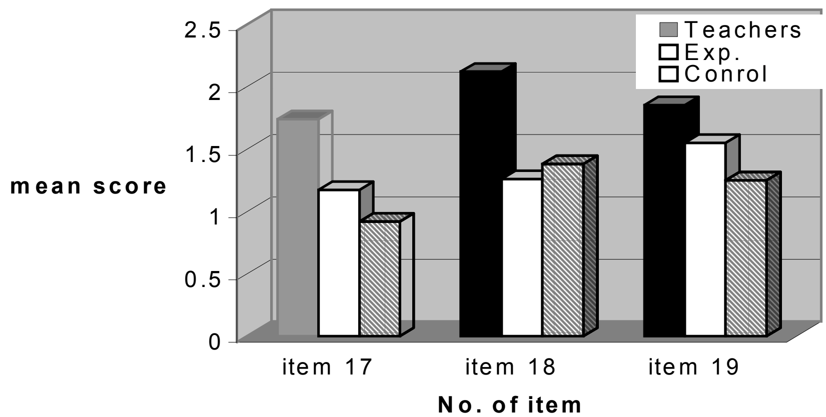


FIGURE. *Mean scores for items 17-19 by research group.*

Students from the control group did not have the same experience, therefore their examples were from various domains, such as: accumulation states, energy levels, models of an industrial plant, and of course models dealing with bonding and structure. Due to the diversity of answers of the control group, it scored higher than the experimental group on this item. From Figure 1 we see that teacher scores were higher than those of the students in both groups. Nevertheless there is still room for improvement in both.

The rate of success for the various categories (1-4) for the experimental group was 70%, 66%, 70%, and 50% respectively. For the control group the corresponding figures were 78%, 46%, 34%, and 32%. These figures show that experimental group students perceived the model concept as expressed by items of categories 2, 3, and 4 better than the control group students. Items of category 1 – models as describing and explaining phenomena – which were relatively straightforward, were correctly perceived by both groups regardless of the learning environment.

While the experimental group students scored better than the control group students in categories 2, 3 and 4 ($p < 0.05$), both had difficulties with category 4, which deals with the ability of a model to explore and predict occurrences. The low score this category got in both groups is due to the fact that the aspects of the model as prediction and research tools were not emphasized in the learning process. Students therefore did not agree with statements claiming that a model does have these exploration and prediction abilities.

The corresponding results for the teachers were: 92%, 61%, 83% and 62%. We see that for the teachers too category 4 was difficult, but also category 2 which dealt with mental models. It points out that there is still work to prepare teachers and widen their model perception.

CONCLUSION AND FUTURE RESEARCH

The results of this study indicate that overall the in-service training program on models put emphasis on many aspects of the trainees' model perception. The importance of the training is that it made teachers realize the role of models and their initial perception of models was expanded. The most significant outcome of the training is reflected in the school implementation, where a noticeable difference between experimental and control groups was found. Experimental group students scored higher than those of the control group in all four score types of the model perception questionnaire. The difference turned out to be significant in the category and the chemistry models parts. This indicates the effectiveness of the treatment on high school students' conceptualizing the meanings of models, especially in the domain of chemistry.

Teachers appreciate the value of models as well as their limitations. Hence, more time should be invested to introduce pre- and in-service chemistry teachers to the model concept and to their use in science in general and in chemistry in particular. More research is needed to determine the long-term effect of such training on participant perceptions and the influence it had on students of the trainee teachers.

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