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Assessing high school chemistry students' modeling sub-skills in a computerized molecular modeling learning environment

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Abstract Much knowledge in chemistry exists at a molecular level, inaccessible to direct perception. Chemistry instruction should therefore include multiple visual representations, such as molecular models and symbols. This study describes the implementation and assessment of a learning unit designed for 12th grade chemistry honors students. The organic chemistry part of the unit was taught in a Computerized Molecular Modeling (CMM) learning environment, where students explored daily life organic molecules through assignments and two CMM software packages. The research objective was to investigate the effect of the CMM learning unit on students' modeling skill and sub-skills, including (a) drawing and transferring between a molecular formula, a structural formula, and a model, and (b) transferring between symbols/models and microscopic, macroscopic, and process chemistry understanding levels. About 600 12th grade chemistry students who studied the CMM unit responded to a reflection questionnaire, and were assessed for their modeling skill and sub-skills via pre- and post-case-based questionnaires. Students indicated that the CMM environment contributed to their understanding of the four chemistry understanding levels and the links among them. Students significantly improved their scores in the five modeling sub-skills. As the complexity of the modeling assignments increased, the number of students who responded correctly and fully decreased. We present a hierarchy of modeling sub-skills, starting with understanding symbols and molecular structures, and ending with mastering the four chemistry understanding levels. We recommend that chemical educators use case-based tools to assess their students' modeling skill and validate the initial hierarchy with a different set of questions.

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Introduction

Symbolic and microscopic representations are frequently used in chemistry textbooks for applying ideas about particles and explaining observations of phenomena. However, many high school students find these representations difficult to grasp and use; they are frequently unable to translate between empirical formulae, electron configurations, molecular structures, and ball-and-stick models (Brosnan and Reynolds 2001; Keig and Rubba 1993). Chemistry instruction should therefore indicate the close connections between visual and conceptual entities and include multiple representations of a specific concept (Barak and Dori 2005; Wu and Shah 2004). Osborne et al. (2003, p. 706) noted: "Students should be encouraged to do science, … to engage in activities such as creating models/pictures to explain ideas… and to consider possible ideas to explain phenomena…"

Based on Osborne and colleagues' recommendation (2003), this study applied representation tools developed for scientists in high school chemistry classes in a specially designed learning environment. We first discuss the difficulties of understanding the chemistry subject matter and the recommended visualization tools that chemical educators can employ in secondary schools and in higher education. We then discuss our learning environment and assignments, which enable students to cope with the microscopic nature of chemistry, and provide an analysis of students' responses to the reflection questionnaire. Next, we present the case-based questionnaires used to assess students' modeling skill and examples of students' responses. We also provide qualitative and quantitative analyses of the modeling skill and sub-skills. Finally, we discuss the hierarchy of modeling sub-skills difficulty level.

Theoretical background

Chemistry can be described at three distinct levels: the macroscopic (sensory) level (visible/touchable phenomena), the microscopic level (atomic/molecular particles), and the symbolic level (representing matter in terms of formulae and equations) (Gabel 1998; Johnstone 1991). A fourth 'process' level was suggested by Dori and Hameiri (2003): at the process level, substances are formed, decomposed, or react with other substances. A student's response is considered to be at the process level when two conditions are fulfilled: s/he demonstrates understanding of the reaction through which a compound is generated, decomposed, or interacts with other compound(s), and s/he is capable of explaining the reaction in terms of one or more of the first three levels. The process level has been implemented as part of a scoring scheme in other studies (Kaberman and Dori 2009; Dori and Sasson 2008) and was instrumental in a paper by Robinson (2003).

Difficulties in learning the chemistry subject matter

Many high school students find it difficult to understand macroscopic changes on the basis of microscopic explanations. The concepts in chemistry involve large quantities of particles that are extremely small in nature, often preventing students from being able to connect a representation of the compounds at the microscopic level with how they are actually structured at the macroscopic level (Gabel and Sherwood 1984; Gabel et al. 1992).

Kozma and Russell (1997) argued that understanding chemistry relies on making sense of the invisible and untouchable. As much of chemistry exists at the molecular level, inaccessible to direct perception, chemistry is inherently representational or symbolic. The researchers raised the question of whether chemistry students understand the communicative intent of the representations used by chemists and modern textbooks, and whether students have the necessary prior knowledge to comprehend chemical principles from images, formulae, diagrams, and graphs.

Nicoll (2003) used five categories to describe the variances observed in how undergraduate chemistry students chose to build a model: arrangement, color, geometry, size, and sticks. The researcher found that students do not necessarily have a developed mental image of how atoms are arranged in a specific molecule, nor do they necessarily pay attention to bonding when building molecular models. Chemists have developed the ability to 'see' chemistry in their minds as images of molecules and their transformations. Chemists also construct, transform, and use a range of symbolic representations: drawings, equations, and graphs (Kozma and Russell 2005). Thus, an important goal of chemical educators is to make students aware of their misconceptions and help them to 'see' chemistry as chemists do, by switching between diverse representations, enabling them to develop scientifically based concepts.

Visualization and models

Visualizations are perceptible, symbolic images and objects in the physical world that are used to represent different aspects of phenomena in order to make the unseen seen (Dori and Belcher 2005; Kozma and Russell 2005). Chemists have developed a variety of representations, especially models, to investigate natural phenomena through the concepts of molecules, atoms, subatomic particles, and the relationships amongst them. A model is a representation of an object, event, process, or system (Gilbert and Boulter 1998), or a physical or computational representation of the composition and structure of a molecule.

Gilbert (2005) discussed model types, including expressed, consensus, scientific, and teaching models. Specially developed teaching models are created to support the learning of some abstract topics, especially concepts related to bonding and structure (Kozma and Russell 2005). Computerized modeling environments and visualization modes may affect the structure of mental models that students acquire during learning and can help students gain better insight into aspects of structure and process in chemistry (Dori and Barak 2001; Schnotz and Kürschner 2008).

Molecular modeling software enables one to interactively construct ball-and-stick, space-filling, and electron density models even for large molecules. Interactive modeling programs provide for the construction of molecules from atoms, find the lowest energy geometric structure, measure bond lengths and angles for this structure, and manipulate and rotate the model to be viewed from different angles (Barak and Dori 2005; Kozma and Russell 2005). Viewing dynamic 3D animations can improve students' incomplete mental models of the dynamic nature of chemical reactions (Sanger et al. 2001).

Representational competence is described by Kozma and Russell (2005) as a set of skills and practices that allow a person to reflectively use representations or visualizations to think about chemical phenomena and processes and to communicate information about them to others.

Using representations to perform tasks requires a series of cognitive operations in the spatial domain, including recognizing the graphic conventions, manipulating spatial information, and mentally tracking constraints. Thus, it is likely that learning chemistry involves visuospatial abilities that enable students to perform cognitive operations spatially, including translating a chemical formula into its molecular structure(s), and visualizing and comparing possible 3D configurations. Being able to comprehend and mentally manipulate chemical configurations is critical for students to conduct advanced scientific research (Wu and Shah 2004).

Unlike content, modeling ability can only be learned through intensive practice, so teachers should teach modeling skills, encourage students to use multiple rather than isolated models, and discuss and critique various models, since each type elaborates only a fraction of its target (Harrison and Treagust 2000, 2001).

Kozma (2003) examined the role of multiple representations in understanding science and found that scientists coordinate features within and across multiple representations to reason about their research and negotiate shared understanding. Students have difficulties moving across multiple representations, so their understanding and discourse are constrained by the surface features of individual representations. The researcher recommended that students use multiple linked representations in the context of collaborative, authentic laboratory investigations.

Dori and Barak (2001) investigated the effect that teaching organic chemistry using virtual and physical models had on students' understanding of both new concepts and the spatial structure of new molecules. They found that experimental students who worked with two kinds of models gained better understanding of the model concept. They were more capable of defining and implementing new concepts and were able to transfer between the chemistry understanding levels: symbol, macroscopic, microscopic and process.

We developed the Case-based Computerized Laboratories (CCL) and Computerized Molecular Modeling (CMM) learning unit, described below, in response to researchers' calls to teach scientific thinking skills, and specifically modeling skill, via multiple representations.

Research objective and design

The research objective was to investigate the effect of the CMM component of the CCL & CMM learning unit on students' modeling skill and sub-skills.

We define modeling skill as understanding of spatial molecular structures and the ability to transfer between molecular representations and chemistry understanding levels. Table 1, the basis of our research design, presents a comparison between the current state of affairs in the literature pertaining to modeling and our study. Based on this analysis, we defined the following modeling sub-skill types: (A) drawing and transferring between a molecular formula, a structural formula, and a model; and (B) transferring between, on the one hand, symbols and/or models and, on the other hand, the microscopic, macroscopic, and process chemistry understanding levels.

Sub-skills of type A require understanding of the symbol level and molecular structure in order to perform transformation among the various chemical representations. Sub-skills of type B require mastery of combinations of subsets of the four chemistry understanding levels.

Table 1 Comparison between previous research on modeling skill and sub-skills and this study

Topic	Modeling skill in the literature	CMM learning environment and modeling sub-skills
1. Features of scientific knowledge Osborne et al. (2003)	The experts stated that scientific knowledge should aim at providing scientific explanations based on models and representations of reality	We responded to Osborene et al., call for presenting science as a multidimensional interaction among the models and empirical observation of the real world
Levy and Wilensky (2009)	Connected chemistry environment is used for teaching the gas laws and kinetic molecular theory and for connecting the macroscopic form of chemical system to the conceptual model, symbolic and physical world	*We constructed science activities that engage students in hands-on modeling assignments, help them to better understand the microscopic and process levels, and improve their modeling sub-skills*
2. Visualization tools for chemists and students Kozma et al. (2000)	The symbolic elements of structural diagrams can be manipulated by chemists in ways that correspond to the structure of molecules and the processes that are used to synthesize them	We based our criteria of model drawing on the types of representations suggested by Kozma et al., namely constituent components, relative arrangement of atoms in space, and bonding between atoms
	Chemists often use TLC, mass spectroscopy and NMR to generate characteristic traces (streaks of color or peaks on a graph) in order to verify their molecular structures and transform nature in a representational sense	CMM and the unit mediate between macroscopic phenomena, learner's experience, and the microscopic world by enabling model presentation of molecules on the screen. *We focused on visualization through CMM, a tool that chemists use for a variety of purposes*
	To visualize the synthesis process, chemists always sketch structures of reactants and products, and draw symbols, arrows, and equations to describe chemical processes	We examined learners' ability to visualize the synthesis of propylene glycol. The students' assignment included reactants and products, partly as molecular formula and partly as models
3. Teaching of modeling skills Harrison and Treagust (2000)	The authors recommended that teachers teach modeling skill, encourage students to use multiple analogical models, and take the time to discuss and critique them	CMM employs a variety of models, including line, ball-and-stick and space-filling. The modeling sub-skills were discussed in class and students wrote down reflection concerning their use of the CMM environment
	The interviewed student drew models, referred to bond order, shape of the molecule and angles between the atoms. His ability to transfer from one model to another was examined	Our rubrics for assessing students' modeling sub-skills were based on similar criteria. *However we also investigated students' ability to transfer from symbols to macroscopic, microscopic, and processes levels*
4. Coding students' responses Nicoll (2003)	Undergraduate students were interviewed while building play-dough models of formaldehyde based on its molecular formula. Students' responses were analyzed by arrangement, color, geometry, size, and sticks. No transformation was assessed	Our rubrics coded four of these areas and identified as different modeling sub-skills. *We also defined transformations between representations as a sub-skill, quantified students' responses, and scored them*

Table 1 continued

Topic	Modeling skill in the literature	CMM learning environment and modeling sub-skills
5. Improving students' modeling skill via visualization tools Wu et al. (2001)	A development of a simplified version of a visualization tool was based on professional tools Students worked together, constructed molecules, and viewed them in three representation types: wireframe, ball-and-stick, and space-filling. Researchers used video recordings, artifacts, interviews, and pre- and posttests High school students' ability to make transformations between 2D and 3D models improved after studying with eChem visualization tool. They developed better understanding of isomers and polarity	The CMM software is used by chemists. The students only used the basic capabilities Research tools were quite similar: a reflection, and pre/post-questionnaires. *We analyzed different aspects in the questionnaires, and also the scores of the different items in each aspect.* We did not emphasize electron dot representation. *Rather, we emphasized model drawing and transformation between the four chemistry understanding levels* We also found improvement in students' modeling skill. *We presented in detail our assessment tools used to examine the extent of students' improvement*
6. Students' difficulties in transferring among multiple representations Wu and Shah (2004)	Multimedia tools address students' alternative conceptions, such as interpreting visual representations at the macroscopic level by surface features. This type of tools integrates multiple symbol systems to demonstrate chemical reactions at the macroscopic and the symbolic levels	CMM was designed to help students make transformations between the symbolic level and the microscopic level. *The teachers taught students the four chemistry understanding levels: macroscopic, microscopic, symbolic and process. Teachers exposed them to criteria for constructing argumentations that include those chemistry levels. We used the chemistry levels in our rubrics as assessment criteria*
	One misconception students exhibit is interpreting chemical reactions as a static process Some students are not able to form 3D mental images by visualizing 2D structures. A design principle for visualization tool is to facilitate identification of depth cues and transformation between 2D and 3D	Our assignments were designed to emphasize the dynamic nature of chemical reactions while encouraging students to incorporate the process level in their explanations. *This helps eliminate the misconception of the static nature of chemical reactions* Our study investigated students' competence of making the transformations between 2D and 3D representations. *We also examined the frequency of appearance of 3D models in students' drawings in response to questions they were asked*
7. Students' difficulties in translation Keig and Rubba (1993)	The authors investigated students' translation between formula, electron configuration, and ball-and-stick models through think-aloud interviews without any specific treatment. Students were unable to translate from model to formula or build a ball-and-stick model from the formula	When the CMM environment was designed, we assumed that the difficulties described by Keig and Rubba (1993) indeed existed *Our treatment was the development and deployment of the CMM environment and learning unit. Our students improved significantly their ability to transfer between molecular formula and spatial models and* vice versa

Differences and additions are in italic

Research setting

The new learning unit in chemistry—CCL & CMM—was developed at the Technion, Israel Institute of Technology. Development of this unit was part of a national reform in chemical education for Israeli high school students, which brought back the laboratory component into the matriculation examination (Barnea et al. 2010). The target population of the CCL & CMM learning unit was Israeli honors 12th grade chemistry students. The honors curriculum in Israel consists of five learning units, and the CCL & CMM unit is an elective unit of these five. The main pedagogical goals of the unit are to expose 12th grade honors chemistry students to an appealing learning environment that attempts to mimic the chemists' research environment and to foster their higher order thinking skills. The thinking skills we investigated included question posing, modeling, inquiry, graphing skills, and transfer (Kaberman and Dori 2009; Dori and Sasson 2008; Sasson and Dori 2006).

Based on the theoretical subjects that had been studied in traditional lessons in 11th grade, which included such topics as energy, acid–base reactions, and sedimentation, our CCL & CMM learning unit involves inquiry-based experiments in the laboratory. Many organic materials, such as benzene, tri-chloro-ethane, and hexane, are no longer permitted for use in Israeli high school laboratories, due to their hazardous nature. This narrows the number of possible organic chemistry inquiry-based experiments. In response to this challenge, we decided to teach organic chemistry in the CMM learning environment, where the students can investigate daily-life organic molecules without handling hazardous materials that might compromise their health. The students studied the CCL part of the learning unit for about 5 months and its CMM part for another couple of months.

Since our article focuses on modeling skill, we present only the CMM part of the CCL & CMM learning unit and environment. The environment included two CMM software packages, which the students downloaded from the Internet: the ISIS-draw from MDL (2000) and the WebLab Viewer from MSI (2000).[1]

Arguably, the two CMM software packages alone are not sufficient. Indeed, the CMM environment setting included three additional elements: well trained teachers, the learning unit, and assignments that were aimed at familiarizing the students with the microscopic and symbolic levels in their explanations.

The ISIS/Draw software enables students to construct molecules by determining the type and number of atoms and the covalent bonds between them according to the bonding rules. It is also possible to draw carbon chains, sugar rings and amino acid molecules, as well as to add different functional groups to the drawn molecules. After constructing the molecule, students are shown its two-dimensional structure. For example, given the formula of lactic acid, $CH_3CH(OH)COOH$, students are asked to construct the molecule using ISIS/Draw. They then view the molecule in 3D using WebLab Viewer (see Fig. 1).

The software enables the transfer of the 3D drawing between three molecular representation forms (line, ball-and-stick and space-filling), the rotation of the molecules, and measuring bond length and angle size between different atoms (Barnea and Dori 1999). Without these activities students do not necessarily develop an accurate mental image of how atoms are arranged in a specific molecule (Nicoll 2003).

Students were asked to investigate the daily-life molecules and tried to make connections between the measurements they took at the microscopic level and the properties of the substances at the macroscopic level. Viewing the line model of the lactic acid, one can

[1] WebLab Viewer was shareware at the time the experiment was conducted.

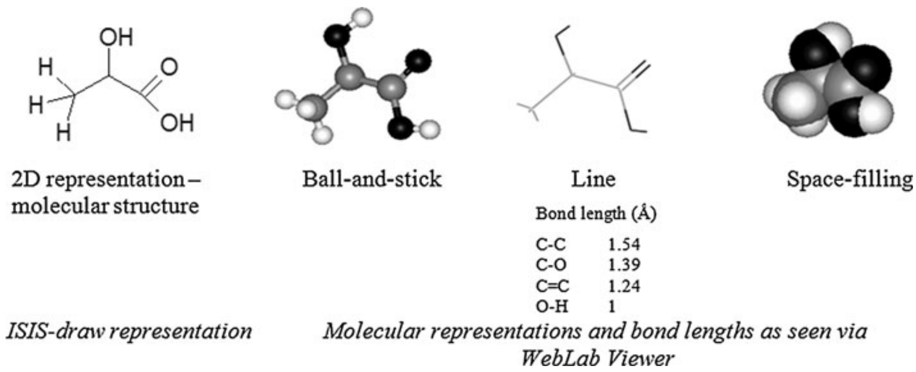


Fig. 1 Four molecular representations of lactic acid

measure bond lengths, but might conclude that it has a planar structure. However, examining the ball-and-stick and the space-filling models shows the spatial structure of the molecule. After investigating the different bond lengths and the functional groups in the molecule, the students were asked to explain (a) the different bond lengths based on the electro-negativity of the atoms and the single/double bonds, and (b) the physical and chemical properties of the substance: boiling point, solubility in water, and chemical reactions. The assignments required an understanding of macroscopic properties and processes of the substance based on the molecule's analysis at the microscopic level.

The students practiced for about 20 hours in the CMM environment and investigated 5–7 different daily-life molecules. They had to construct the molecules and present them in 2D and 3D representations.

Research participants

The research described in this article was part of a longitudinal 3-year project that investigated studying in the CCL & CMM environment. In the first year of the research (first stage), only the CCL part of the learning unit was taught. The first year study findings are described in Dori et al. (2004). A year later, the CMM portion became an integral part of the larger learning unit, and our research consisted of two additional stages (second and third), each spanning a whole academic year. The 614 honors 12th grade chemistry students who studied the CCL & CMM unit were from high schools in Israel. The students (second stage—224 students, third stage—390 different students) underwent the same learning process in the CMM learning environment.

In 10th and 11th grades, these students had studied a variety of topics in chemistry with emphasis on chemical structure and bonding. While designing the learning unit we assumed that the students had this prior knowledge.

The teachers of the research group participated in a summer training workshop and were familiar with the CCL & CMM learning unit and its characteristics. These teachers also participated in an ongoing training throughout the academic year. They received further help and answers to any questions that were raised while they taught the new CCL & CMM learning unit.

To analyze the effect of the students' academic levels on their modeling skill scores, we divided the participants using Duncan's multiple range test into three academic levels—

low, intermediate and high—based on their total pre-questionnaire scores. The total score of the pre-questionnaire was calculated based on average scores of all the thinking skills examined in the CCL & CMM learning unit—modeling, question posing, inquiry, graphing and transfer skills (Kaberman and Dori 2009; Dori and Sasson 2008; Sasson and Dori 2006).

Research tools

We used a mixed method of both qualitative and quantitative research tools (Denzin and Lincoln 2000; Johnson and Onwuegbuzie 2004) to gain deeper understanding of the students' modeling skill. This approach adds insights and understanding that might be missed when only a single method is used (Strauss and Corbin 1990).

As a qualitative research tool, we used a reflection questionnaire, in which we asked students to express their opinions about the CCL & CMM learning unit. We used pre- and post-questionnaires as both qualitative and quantitative research tools to assess students' higher order thinking skills in general and the modeling skill in particular. Initially, the questionnaires underwent content analysis to determine categories based on students' responses. Then, quantitative analysis was applied for descriptive and more advanced statistics.

The reflection questionnaire included six aspects of learning and assessment via the new learning unit, and was administered after completing the learning process in the CCL & CMM learning environment.

The pre- and post-questionnaires were administered to the students before and after the entire CCL & CMM learning unit, respectively. The questionnaires included a case study concerning a chemistry-related real-life story and a variety of assignments for investigating the various thinking skills. One chemical case study from the second stage questionnaire started with the question: *Trees cause air pollution—Is this possible?* It described the substance isoprene (C_5H_8) as the most common organic compound that oak and sycamore trees emit at daylight.

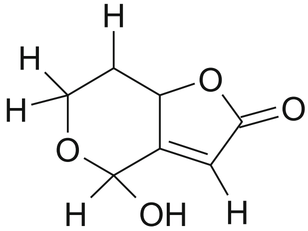
The task that examined modeling sub-skills included five questions. [The text enclosed in brackets is the required modeling sub-skill, which did not appear in the questionnaire.]

1. The molecular formula of isoprene is C_5H_8. Write a possible acyclic structural formula for the molecule. [Transfer from molecular formula to structural formula—a sub-skill of type A.]
2. Draw a model for the structural formula of C_5H_8 you suggested. [Transfer from structural formula to a 3D model drawing—a sub-skill of type A.]
3. Many organic compounds are considered as air pollutants. One of them is propylene (propene), which reacts with water and $KMnO_4$ to produce propylene glycol (3D model is given).

a. Write the molecular and structural formula of propylene glycol. [Transfer from a 3D model to molecular and structural formula—a sub-skill of type A.]
b. Draw a model for propylene. [Transfer from molecular formula to a 3D model drawing—a sub-skill of type A.]

Question 3 required the students to demonstrate their sub-skill of transferring from a 3D model to molecular and structural formulae and vice versa.

4. The structural formula of patulin is described below. Explain in bonding and structure terms why the patulin is solid in room temperature. [Transfer from symbols to macroscopic and microscopic level—a sub-skill of type B.]



5. NaI is a white solid substance, whose molar mass is 150 g/mol with melting temperature of 662°C, while the molar mass of patulin is 154 g/mol, with melting temperature of 110°C. Describe the melting processes of NaI and patulin. Explain the difference between these two processes. [Transfer from the symbol level (structural formula and ionic formula) to the process level expressed as verbal explanations—a sub-skill of type B.]

Question 5 required the student to compare an ionic substance—NaI to an organic substance—patulin. Ionic materials were encountered in the hands-on CCL, while organic materials were the focus of the CMM learning unit.

Some of the modeling sub-skills appeared in both research stages while others appeared only in one or the other (e.g., Questions 4 and 5 appeared only in the third stage which dealt with the *patulin toxin* case study). In addition, the students were allowed to choose not to respond to all the assignments in the questionnaire. They were instructed to respond to at least one question in each of the higher order thinking skills that we examined.

As noted, the students in second and third stages underwent the same learning process in the CMM learning environment. Our questionnaires, administered to both stages, examined five different higher order thinking skills studied in the CCL & CMM unit. One of them was the modeling skill and its sub-skills. Due to the large number of skills and sub-skills we wished to examine, it was not feasible to dedicate a question to each sub-skill in any one of the two stages. Therefore, only a subset of the questions in the two stages examined the same modeling sub-skills. Since the concept and design of the questionnaires in both stages were the same and the intervention program was identical, we combined the responses from the two stages to questions that examined the same sub-skills. Therefore, the results presented in Fig. 3 and Table 3 vary in the number of students.

Assessment of students' responses to modeling skill assignments

New assessment tools were designed especially for the CCL & CMM learning unit in order to encourage the development of students' higher order thinking skills. These assessment tools consisted of a detailed rubric for each skill that enabled us to diagnose students' different thinking skills. Using our rubrics and applying content analysis on students' responses, we categorized the responses to the examined thinking skills and normalized the scores to a 1–100 scale for each skill. The questionnaires were analyzed in two phases. In the first, qualitative, phase we applied content analysis of students' responses to extract categories and used them to characterize students' responses. In the second, quantitative, phase we scored each student's response using the rubrics and statistically analyzed the results. Scoring students' answers to the examined skills in the pre- and post-questionnaires provided us with a broad picture of the students' thinking skills before and after studying the CCL & CMM learning unit.

Examples of students' responses to the assignments, which examined the different modeling sub-skills and their analysis, are presented in Fig. 2.

Findings

A key question in the reflection questionnaire was "In what ways did the CCL & CMM learning unit contribute to deepening your knowledge in chemistry? In your opinion, will the knowledge and skills you acquired during studying this learning unit assist you in the future?" No question instructed the students to specifically relate to the CMM environment or modeling skill. Nevertheless, over 60% of the students referred to the CMM part of the learning unit.

Students reacted positively to CMM and recognized the importance of modeling both to their chemical understanding and to their future career. They noted the advantages of the environment and indicated their enjoyment of viewing and drawing the molecules.

Students' reflections on CMM and modeling skill are introduced in Table 2.

Students' modeling skill was assessed as the sum of the modeling sub-skills described above. We first present a statistical analysis of students' modeling skill scores sorted by academic levels and then the specific sub-skill's difficulty.

In the modeling skill (the sum of all the modeling sub-skills), students' average pre- and post-questionnaire scores in the second stage ($N = 224$) were 48 and 81, respectively, and in the third stage ($N = 390$) 43 and 75, respectively.

The net gain, defined as the post- minus the pre-questionnaire scores, was about 30 points for both stages with no statistically significant difference between the stages. Indeed, the concept and design of the questionnaires in both stages were the same and the intervention program was identical. Therefore, we combined questions that examined the same sub-skill in both stages.

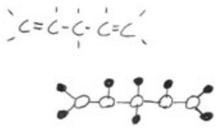
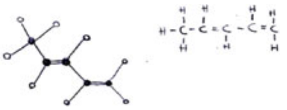
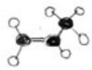
The effect sizes of the net gain scores were statistically significant in both stages ($p < 0.0001$), amounting to 1.17 in the second stage and 0.85 in the third. Table 3 presents students' modeling skill scores by academic level for the two stages.

In both stages, students at all academic levels improved their modeling skill scores significantly. Low academic level students' scores were the highest, implying that, compared with their intermediate and high academic level peers, their modeling skill improved the most, probably due to the ceiling effect.

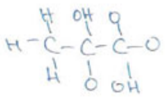
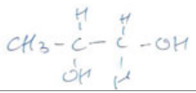
Students' Modeling Sub-Skills Analysis

Content and quantitative analyses of students' responses indicated that the modeling sub-skills were at different complexity levels. The findings are presented next in increasing sub-skill complexity assignments and classified into one of the two modeling sub-skill types: (A) drawing and transferring between a molecular formula, a structural formula, and a model, and (B) transferring between symbols and/or models on the one hand and the microscopic, macroscopic, and process chemistry understanding levels on the other.

A

Modeling sub-skill A	Student's response	Analysis
Transfer from molecular formula to structural formula – question 1 Type A	An insufficient response – student B. 	All bonds and atoms in the structural formula match the molecular formula and the bonding rules (score 2). There is a good representation of atoms in the drawn model but reference to angles and spatial representation is incorrect and there is no distinction between single and double bonds (score 0 – two mistakes). There is only partial match between the structural formula and the model (score 1).
Transfer from structural formula to a 3D model drawing – question 2 Type A	A high level response – student D. 	All the bonds and atoms in the structural formula match the molecular formula and the bonding rules (score 2). A correct model with correct angles that make the distinction between 2D and 3D is drawn, and a distinction is made between single and double bond (score 2). There is a complete match between the structural formula and the model (score 2).
Transfer from molecular formula to a 3D model drawing – question 3c Type A	An incorrect response – student L. 	The number of carbon and hydrogen atoms suits the molecular formula of C_3H_6, but there is no reference to the bonding rules. Propene is an alkene and a double bond has to be drawn. Reference to angles and spatial representation is incorrect (score 0). The student did not write a structural formula before drawing the model and the transfer he made was incorrect (score 0).
	A high level response – student O. 	A correct model with correct angles that make the distinction between 2D and 3D is drawn, and a distinction is made between single and double bond (score 2). There is a complete match between the structural formula and the model (score 2).

B

Modeling sub-skill A	Student's response	Analysis
Transfer from a 3D model to structural formula – question 3b Type A	An incorrect response – student F. 	The student confused between hydrogen and oxygen atoms, and made more than two mistakes when transferring from the model to the structural formula. The student drew the formula without noticing the bonding rules, the oxygen atoms on the middle and right carbon atoms are missing one bond (score 0).
	A high level response – student N. 	A complete linkage between the model and the structural formula, a correct structural formula for propylene glycol (score 2).

Modeling sub-skill B	Student's response	Analysis
Transfer from symbols to macroscopic and microscopic level – question 4 Type B	A high level response – student Y. *Patulin is a molecular substance, made of molecules which are held together by intermolecular interactions. The stronger those interactions are, the closest to each other the molecules are, and the solid state is obtained. The intermolecular interactions between patulin molecules are hydrogen bonds and Van der Waals interactions. Because of the oxygen atoms presence and the high molecular weight, the Van der Waals interactions are strong. In room temperature, patulin molecules are packed closely and the substance is solid.*	The three factors that affect the state of matter were mentioned and correctly explained (score 2).
Transfer from the symbol level (structural formula and ionic formula) to the process level accompanied by verbal explanations – question 5 Type B	A high level response written by student K. *NaI is built of ions with strong interactions between them because of the electrostatic forces between cations and anions, while between patulin molecules hydrogen bonds and Van der Waals interactions. When reaching the melting point the intermolecular bonds break. The ionic NaI bonds are stronger and the melting point is higher. When ionic bonds break, the melting substance contains mobile ions.*	The student made a distinction between the structures of the two substances, identified the intermolecular bonds and consequently could explain the difference in the melting temperatures (score 2).

Fig. 2 Analysis of students' responses to modeling sub-skills Type A & B assignments

Table 2 Categories gleaned from students' responses to the reflection questionnaire

Categories	Examples
Transfer between levels of chemistry understanding	W: I learned visually about molecular structures. Using a picture, drawing, or sketch I was able to understand processes at the microscopic leve
A computerized environment	R: … Because of the integration of computers into the unit, I enjoyed performing experiments and explore molecules via molecular modeling
An enjoyable environment	EI: I enjoyed drawing the molecules and really see the molecule I learn about. I enjoyed working on the molecule inquiry project and investigating an interesting molecule on my own
Inquiry	O: I liked the molecule inquiry project, as this assignment made it possible for me to choose a molecule of a substance I am familiar with from daily life and which I was curious to investigate
Contribution to future professional career	M: I want to study Genetics in the future, and this requires intensive work with computers and models of different DNA molecules. The skills I acquired will help me build 3D models of molecules and better understand the research I will be conducting
Connection to previous chemistry topics	A: In molecular modeling activities, we examined bond lengths and types. These activities enabled us to better understand subjects which we had studied theoretically two years earlier and took for granted what was written in textbooks without any proof
Spatial ability	I: The learning unit improved my spatial ability to visualize how a molecule of a substance looks like and my ability to analyze it. Till now I could only imagine the molecules by looking at plastic models or drawing the structure formula, but not spatially. Now I can see each particle and the way it is bonded to other particles

Table 3 Students' scores in the modeling skill sorted by academic levels and stages

Academic level	$\bar{x}$ Second stage					t*	$\bar{x}$ Third stage					t*
	N[a]	Pre	SD	Post	SD		N[a]	Pre	SD	Post	SD	
High	42	63	22	88	16	5.8	143	51	23	74	18	8.6
Intermediate	137	43	25	77	20	13.6	184	39	22	75	19	13.4
Low	45	46	28	86	14	8.8	49	35	18	76	19	9.8
Whole population	224	48	26	81	19	17.0	376	43	23	75	19	16.6

*$p < 0.0001$

[a] $N_{total} = 600$ for the academic level analysis, since only students who responded to both questionnaires were considered

Figure 3 presents students' performance in four of the five examined modeling sub-skills—two of type A and two of type B. The first task, depicted in the upper left graph, relates to transferring from molecular to structural formula:

The molecular formula of isoprene is C_5H_8. Write a possible acyclic structural formula for the molecule.

In this sub-skill, already in the pre-questionnaire, 75% of the students transferred from the molecular to the structural formula correctly. This number increased to 86% in the post-questionnaire.

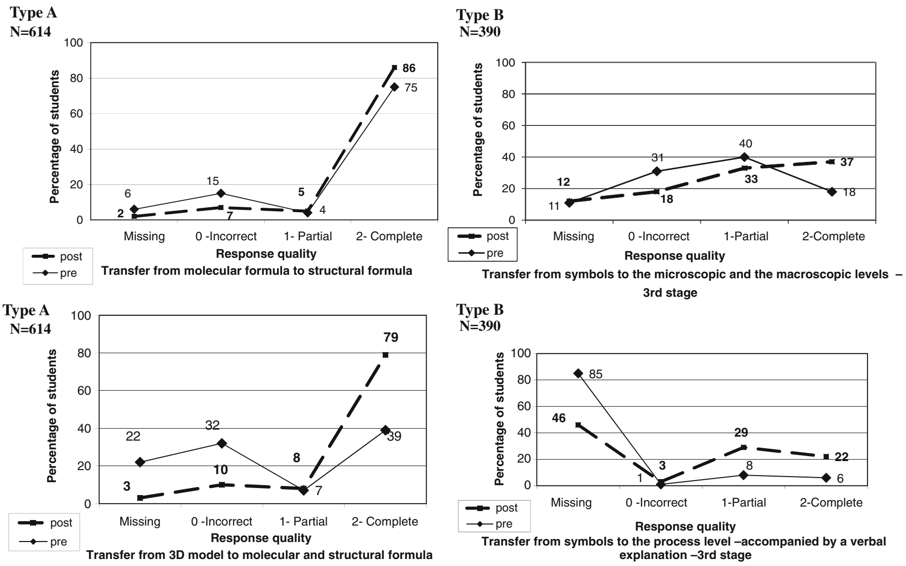


Fig. 3 Distribution of students' performance in Type A & B assignments

The second sub-skill was transfer from a 3D model to molecular and structural formulae. The assignment here aimed to assess how students convert an unfamiliar 3D model into its molecular and structural formulae: "Write the molecular and structural formula of product 1—propylene glycol." The students had not only to know the atoms involved, but also to understand the whole structure of the molecule. The results, shown at the bottom-left corner of Fig. 3, were that in the pre-questionnaire, 22% of the students did not respond to the assignment at all, 32% of them wrote an incorrect response, and 7% made a partial transfer from the model to the molecular and structural formula. In the post-questionnaire, only 13% of the students did not respond or gave an incorrect response. The percentage of students who provided a complete response, implying that they succeeded in making the transfer from the 3D model to the molecular and structural formula, doubled from 39% in the pre-questionnaire to 79% in the post-questionnaire.

The third sub-skill examined, transfer from simple and complex molecular formulae to a model, was designed to examine how students draw a model from simple and complex molecular formulae. It included two assignments: Draw a model to the substance propylene (propene), C_3H_6; and Draw a model for the structural formula of C_5H_8 you suggested in question 1.

Propylene (C_3H_6) is a relatively simple molecule, while isoprene (C_5H_8) is more complex, as propylene contains only three carbon atoms and one double bond, whereas isoprene contains five carbon atoms and students can place its two double bonds in various combinations or draw a model with a triple carbon–carbon bond. We compared the post-questionnaire frequencies of model types students had generated in response to the two assignments to their pre-questionnaire responses (see Table 4).

In the pre-questionnaire, half of the students did not draw any model, most likely because they were given the option not to respond to all the questions. In the post-questionnaire, 88% of the students at least tried to draw a model, indicating a huge increase in their confidence in drawing models. There was a threefold decline from the pre-questionnaire (22%) to the post-questionnaire (7%) in the percentage of students who drew

Table 4 Distribution of students' performance in 3D model drawing and transfer assignments

Response quality ($N = 614$)	Percentage			
	Model drawing		Transfer from structural formula to 3D model	
	Pre	Post	Pre	Post
Missing	50	12	50	12
Incorrect	8	6	10	5
Partial	29	36	3	7
Complete	13	46	37	76

linear 2D models and a parallel threefold increase in drawing spatial models (from 26 to 80%). Further analysis of transferring from molecular and structural formulae to a 3D model is based on our rubrics of the drawing sub-skill, which were based on the quality of the simple and the complex molecular models students drew.

While in the pre-questionnaire about half of the students did not respond or drew an incorrect model of the molecule, the analogous percentage decreased to less than a quarter in the post-questionnaire. With respect to the quality of the models of the molecule, as shown in Table 4, 46% of the students drew the model correctly in the post-questionnaire, compared with only 13% in the pre-questionnaire.

In the post-questionnaire, most (76%) of the students who were able to transfer from the formula to the model did so correctly, and only 7% made a partial transfer, while in the pre-questionnaire only 37% of the students succeeded in making a complete transfer and 3% made a partial one.

The fourth sub-skill, transfer from the symbol to the microscopic and macroscopic levels—type B modeling sub-skill (given in the third stage only and depicted in the top-right of Fig. 3)—was examined by the following assignment: The structural formula of patulin is described below, explain in bonding and structure terms why the patulin is solid in room temperature.

About 10% of the students skipped this assignment in both the pre- and post-questionnaires. In the pre-questionnaire, 70% referred to the question incorrectly or partially, while in the post-questionnaire only 50% responded incorrectly or partially. The percentage of students who responded fully doubled from the pre- to the post-questionnaire.

The fifth, last, and most complex examined modeling sub-skill was transfer from the symbol to the process level. Requiring textual explanation, this type B sub-skill was examined via the following assignment: Describe the melting process of NaI and of patulin. The outcomes are presented in the bottom-right of Fig. 3.

This assignment was indeed found to be the most difficult, as it requires utilizing and transferring through all four chemistry understanding levels, from the symbols of patulin and NaI to their melting processes.

While only a small percentage of the students (15%) responded to this difficult task in the pre-questionnaire, 54% at least attempted to perform this assignment in the post-questionnaire ($N_{total} = 390$ students).

Discussion

This research concerns the higher order thinking skill of modeling and modeling sub-skills, as employed by students coping with multiple representations, reactions, and physical properties of organic compounds. We have established that the CMM learning environment contributed to improved modeling skill scores for students at all academic levels. In what follows, we discuss our findings regarding students' different modeling sub-skills, ordered in increasing level of difficulty. We then look into students' achievements in the modeling skill as a whole, based on the sum of their modeling sub-skills scores.

Transfer from molecular formula to structural formula

The ability to transfer from a molecular to a structural formula does not necessarily require exposure to the CMM environment, as students regularly study transfer from molecular to structural formula in traditional organic chemistry classes. Since all the students who took the pre-questionnaire in the beginning of 12th grade had already been examined on organic chemistry in their 11th grade matriculation test, we expected the students to provide a correct response to this task regardless of their inclusion in our research group. Indeed, about 75% of the students already correctly transferred from molecular to structural formulae in the pre-questionnaire. In the post-questionnaire, more than 80% of the students made a complete transfer and suggested a correct structural formula to the given molecular formula.

Transfer from a 3D model to molecular and structural formula

The propylene glycol assignment required the students to count the number of different atoms, each presented with a different color, and to understand the structure of each molecule and the bonds between the molecule's atoms. In the pre-questionnaire, about half of the students did not answer this question or answered it incorrectly, while about 40% answered it correctly. In the post-questionnaire, about 80% of the students correctly transferred the 3D model into molecular and structural formulae.

While engaged in CMM-based investigation of different molecules, students constructed their 2D structural models and transferred them to 3D models. This gave them a feeling for the correspondence between the molecular formula, the structural formula, and the 2D and 3D models of the same molecule. It is therefore unsurprising that in the post-questionnaire 79% of the students made a complete transfer from the model of propylene glycol to its structural formula, compared with only 39% in the pre-questionnaire. Wu et al. (2001) also reported that high school students' ability to make transformations between 2D and 3D models improved after studying with eChem, a computer-based visualization tool.

Model drawing of simple and complex molecules

In the pre-questionnaire, about half of the students did not draw any model, while in the post-questionnaire, 82% drew models, indicating an increase in their confidence to draw models (see Table 4). Initially, the students were not familiar with the model drawing task, since drawing models in general, and 3D models in particular, had not been emphasized in class, and the teacher was the only one who drew 2D structural formulae on the board. It was only after the teachers had participated in the training program, conducted to assimilate the learning unit, that they became aware of the need to draw 3D models and to teach this skill to their students. Teachers' professional development is indeed key to incorporating visuospatial models into science teaching. This necessary professional development can be achieved through teacher preparation and in-service programs. De Jong et al. (2005)

claimed that pre-service chemistry teachers need to develop pedagogical content knowledge about using particle models to help secondary school students understand the relationships between phenomena and corpuscular entities. In our post-questionnaire, only about 10% of the students did not try to draw a model, indicating that most students felt comfortable performing this type of assignment.

In the post-questionnaire, about 80% of the students drew ball-and-stick models, but a very few (one or two) students chose to draw 3D space-filling models. Our findings agree with those of Wu et al. (2001), who argued that students do not prefer space-filling models in identifying structural differences and functional groups because bond types (i.e., single, double, or triple) are invisible in this type of model. The ball-and-stick models are most concrete, because they convey the visible information of atoms and bond orders. It is also more difficult to draw 3D space-filling models by hand due to the need to express 3D information on two dimensional paper without any computer assistance.

We assessed the model drawings from two aspects: (a) drawing quality in terms of bonds, angles, and linear vs. spatial expression, and (b) the quality of transfer between the structural formula that the students suggested and the model they drew, as well as the extent to which they understood the linkage between the two, as expressed by matching the kind and number of atoms and the covalent bonds between them.

Almost half (46%) of the students in the post-questionnaire drew correct and complete models, making the distinction between single and double bonds and drawing correct angles that gave the model its spatial characteristics, compared to only 13% who drew a correct and complete model in the pre-questionnaire—a 3.5 factor increase.

The students utilized the CMM environment to conduct a long inquiry process, in which they investigated several molecules by viewing them in three kinds of 3D models. The teachers used the CMM environment to focus on spatial molecular structures in class discussions, referring to measurements of angles between different atoms that the students had taken, such as the 109.5° angle between a carbon atom and two atoms attached to it, typical of tetrahedral structures.

Most of the molecules students investigated were organic compounds. We expected students to draw their models in the post-questionnaires in a way that resembled what they had seen on the computer screen. Yet there were students who drew linear models with no spatial characteristics. We attribute this to the fact that the assignments students had to submit before they responded to the post-questionnaire were mostly computerized, and the students printed screenshots as responses. Therefore, they did not have enough practice in drawing models using paper and pencil. This might explain difficulties encountered by about half of the students in drawing spatial models in the post-questionnaire.

Transfer from symbols to the microscopic and macroscopic level

The percentage of students who responded correctly to the assignment calling for transferring from symbols to the microscopic and macroscopic level doubled from the pre- to the post-questionnaire. Student O. wrote: "The learning unit contributed to my understanding of the symbolic level. Through molecular modeling I could see the molecules [*microscopic level*] I investigated in different forms of representation, beyond the letters [*symbolic level*] which represent the molecule. It contributed to my understanding of substances properties [*macroscopic level*]."

In spite of this improvement, only 37% of the students in the post-questionnaire referred correctly and fully to the different aspects of the inter-molecular interactions between the patulin molecules. Most of the students identified the hydroxyl functional groups in the structural formula of the patulin, but ignored its high molar mass and the electronegative oxygen atoms, two additional factors that strengthen the inter-molecular Van der Waals interactions. Many students referred to the covalent bonds between the atoms, indicating lack of comprehension of the factors that affect the state of the matter.

The assignments that accompanied the visualization activities in the CMM learning unit emphasized the connections between the symbolic, macroscopic, microscopic, and process levels. Assisted by the ISIS-draw and the WebLab Viewer software packages, students investigated the molecules according to guiding questions in the unit. Teachers conducted intensive class discussions about the physical properties of the substance and the inter-molecular interactions that affect them. However, after this treatment students still experienced difficulties in transferring between the symbolic level and the microscopic and the macroscopic levels. This finding resonates with that of Brosnan and Reynolds (2001), who noted that although symbolic and microscopic representations are frequently used in chemistry textbooks, applying ideas of particles and constructing microscopic representations to make explanations of observations are difficult for many secondary school students. Indeed, while the CMM learning unit did improve students' capabilities to transfer from the symbolic to the micro and macro chemistry understanding levels, there is room for further improvement, and planning needs to be done to increase students' achievements in this sub-skill.

Transfer from the symbol to the process level with verbal explanation

The assignment designed to examine this sub-skill involved symbols of the ionic NaI compound and the molecular patulin compound, whose structural formulae was given. Students had to describe and write for each of the substances its melting process equation. In order to respond to this task correctly, students had to transfer from the lower symbolic level to the highest, process level, the highest of the four chemistry understanding levels. While making this transfer, they had to traverse the intermediate microscopic and macroscopic levels. During the teachers' training program we emphasized the significance of constructing proper argumentations based on the chemistry understanding levels. A good argumentation should contain as many as possible of the four chemistry understanding levels, since an argumentation that is based on the various levels would include all the relevant chemical and/or physical aspects.

Not surprisingly, the transfer from the simplest symbol level to the most advanced process level was the sub-skill that students found the most difficult. Even in the post-questionnaire, 46% of the students elected not to respond to this task, but this was almost half the percentage (85%) of those who elected not to respond to this question in the pre-questionnaire. However, of the respondents in the post-questionnaire, 94% provided a partial or a complete answer. The relatively low student response rate compared with the response rate to other questions, as well as the partial responses, exposed various hurdles, such as an inability to identify NaI as an ionic substance or to explain the melting process of patulin as breaking intra-molecular covalent bonds. Bonding and structure is one of the most important subjects in the chemistry curriculum in Israel, but high school students, both in Israel and around the world, still lack fundamental understanding of chemical bonding (Levy Nahum et al. 2007). In view of this finding, we recommend that teachers spend more time with their students on transferring from the symbol to the process level and develop well-structured argumentations that include at least three of the four levels of chemistry understanding. Such argumentations will enable students to regulate their

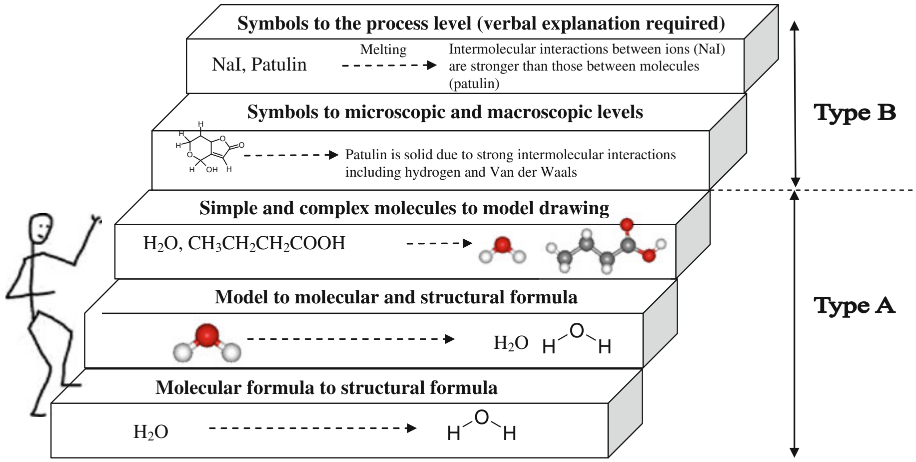


Fig. 4 Hierarchy of the modeling sub-skills

learning and check whether their answers are complete, while the teachers will be better equipped to identify students' misconceptions and to correct them.

The various modeling sub-skills are presented pictorially in Fig. 4 as a hierarchy of increasing difficulty. As the student climbs the steps, s/he is required to master increasingly higher level modeling sub-skills, starting with transferring from molecular to structural formula at the bottom, all the way to transferring from the symbol to the process level. Each stair contains the modeling sub-skill definition, while the vertical face of the stair has an example of the sub-skill taken from the questionnaire.

The CMM learning environment facilitates the development of students' abilities to transfer among molecular representations and chemistry understanding levels, all the way from the symbol level to the process level. At the bottom of the hierarchy, a student is required to transfer from understanding a symbol of a molecular formula of a single molecule to its structural formula. At the top of the hierarchy, the student should be able to explain the melting processes of both ionic and molecular substances and to compare the two.

Overall achievements in the modeling skill of the CMM students

To obtain a general modeling and transfer score, we totaled each student's scores in each modeling sub-skill. In both stages of the study, the students improved their modeling skill achievements significantly. The average starting point was quite low, with a pre-questionnaire average score of less than 50 in both stages.

In the pre-questionnaire students had not yet been exposed to the CMM environment, neither had they practiced transfer between models and formulae. Their knowledge in organic chemistry was acquired a year earlier, during 11th grade, as they were working occasionally with plastic models. After exploring molecular models in computerized media, students became more skillful in writing structural formulae of molecules, drawing models spatially, making connections between the different representations of molecules, and using the different levels of chemistry understanding—symbol, microscopic, macroscopic, and process—for their argumentations.

To gain deeper insight into the students' total modeling skill, we divided them into low, intermediate, and high academic levels. The findings in both stages were consistent and showed that students in all academic levels improved their scores significantly. Comparing the net gain scores of each one of the three academic level students, we found that low academic level students improved the most, while high academic levels students improved the least.

Students at a low academic level usually find it difficult to understand the microscopic level of chemistry and to imagine the abstract structure of the molecules. The learning process in the CMM environment is most useful for these students, as it simplifies the microscopic level and provides views of diverse representations of molecules, which had been invisible. The students can also manipulate the molecules and observe them from different angles, measure different parameters and investigate them in new ways. At the end of the process, students' scores in all academic levels were very similar and the gap between them was narrowed.

High academic level students had good spatial abilities and needed the training provided in the CMM environment less than the low academic level students. Due to the ceiling effect, their net gain was the lowest. As Small and Morton (1983) showed, direct training or practice on visuospatial tasks can improve achievements in chemistry. Students who received training on visualization skills had significantly higher scores on questions that required the use of 3D models in a retention test.

The net gain scores of the students in the modeling skill were high, about 30 points on average, and were consistent over the 2 years (see Table 3). We attribute this outcome to two aspects: (1) the intensive process that the students underwent while responding to variety of learning tasks in the CMM environment; and (2) the teachers who participated in summer training programs and received on-going support throughout the academic year.

The modeling skill with its sub-skills is one of several higher order thinking skills examined in our longitudinal study. As Zohar (2004) claimed, while many science teachers maintain that only high achievers should be taught to acquire higher order thinking skills, students of all academic levels can benefit from such teaching. Our findings support this claim.

Research limitation, strengths, and recommendations

Our research has one limitation and several strong points, as well as contributing to the knowledge base of students' comprehension of models and transfer among different representations of molecules.

The research limitation is that some of the sub-skills were assessed by only one question. These questions may not be the sole representatives of their respective sub-skill. However, there is a limit to the length of a questionnaire one can require students to complete. We propose an initial hierarchy based on our findings. Future research should validate this hierarchy through additional assessment.

Beside this limitation, the research features the following strengths:

- We defined a new set of sub-modeling skills (types A and B), ranked it, and suggested an initial hierarchy of their difficulty levels. Type A sub-skills are related to drawing and transferring between a molecular formula, a structural formula, and a model. Type B modeling sub-skills deal with transferring between symbols and/or models on the one hand and the microscopic, macroscopic, and process chemistry understanding levels on the other hand. The two modeling sub-skill types were found to be intertwined, with sub-skills of type A being in general lower than those of type B. We recommend that teachers become aware of the various modeling sub-skills and their hierarchy.

- New assignments and case-based tools were developed, and the content of students' responses was thoroughly analyzed. Other researchers can validate our initial hierarchy using a different set of questions.
- We have established a connection between students' modeling skill and their ability to understand and explain chemical phenomena via the four levels of chemistry understanding. Since textbooks often use a variety of models and symbols, students are expected to be competent in transferring between the symbol level and the macroscopic, microscopic, and process levels. The CMM learning environment and the corresponding teaching approach can be most instrumental in facilitating this transfer.

Russell and Kozma (2005) argued that test items requiring students to supply answers are more likely to cause them to look beyond the surface features of the visualizations and produce responses based upon their views of the underlying chemistry. Our case-based questionnaires responded to this call while focusing on CMM visualization, a tool that chemists use. By presenting our assessment tool and its content analysis for modeling sub-skills assignments, we present teachers and educators with ways to analyze their students' responses both qualitatively and quantitatively. The assessment tools were found to be diagnostic, as we were able to pinpoint specific difficulties in drawing 3D models and in transferring amongst the four levels of chemistry understanding.

Finally, student improvement was most noticeable amongst the low academic level students. This might indicate that the CMM environment provides adequate scaffolding, especially to the lower achievers. Last but not least, this study ranks important sub-skills within the modeling skill.

In view of the value of fostering students' modeling sub-skills, we recommend that chemical educators use case-based tools to validate the initial hierarchy with a different set of questions.

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