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A Student Evaluation of Molecular Modeling in First Year College Chemistry

Julie B. Ealy[1]

This three-year study involved an evaluation of molecular modeling by students in first year college chemistry. The molecular modeling program utilized was Spartan (Wavefunction, Inc., Irvine, California) on a UNIX-based platform with Silicon Graphics Indigo series workstations. A treatment group of 129 students visited a computer room four times during the semester for two-hour sessions. They completed exercises on periodic trends in atoms, structure of molecules, electronic structure of molecules such as MO and valence bond theory, and properties of organic molecules. The students were required to complete an evaluation of the molecular modeling computer experience at the end of the semester regarding aspects such as: effectiveness, integration with course content, interest, benefit, and advantages and disadvantages. Also obtained through the evaluation were students' opinions regarding the helpfulness of the molecular modeling computer experience for 3-D visualization of atomic and molecular structure and whether their understanding of atomic and molecular structure was enhanced. The first two years of the study constituted a pilot study and data for this study were obtained in the third year. Though the specifics are not reported here, quantitatively the achievement of the treatment and non-treatment groups was also assessed. There was a significant difference in achievement on the Final Exam of the semester ($p = 0.0067$) between the treatment and non-treatment groups on multiple choice questions pertaining to concepts of resonance, dipole moment, and atomic/molecular stoichiometry.

KEY WORDS: Evaluation; molecular modeling; first year college chemistry.

INTRODUCTION

In the Fall of 1995, the Edison Project for Communicating Chemistry initiated a three-year project. It was designed to test the proposition that sophisticated molecular modeling software could be usefully integrated into first year college chemistry. Likewise, could ChemGate serve as a model for introducing students to a computer application that normally they not would see until later in their science experience, if at all? The name ChemGate was derived from the role played by the NSF-funded Gateway Coalition which provided support. During the first two years, which constituted a pilot study, the students met in the Gateway lab of the Engineering building. In the third year they met in a computer lab in the Chemistry building where data for this study were collected concerning students' evaluative opinions of the computer application (Ealy, 1998).

The molecular modeling program utilized was Spartan (Wavefunction, Inc., Irvine, Calfornia) on a UNIX-based platform with Silicon Graphics Indigo series workstations. The treatment group consisted of 129 students who visited a computer room four times during the semester for two-hour sessions. They completed exercises pertaining to periodic trends in atoms, structure of molecules such as bond angle and bond length comparisons, electronic structure of molecules such as MO and valence bond theory comparisons for the same molecules, and properties of organic molecules. The students were required to

[1]Columbia University/Rye Country Day School, Havemeyer Hall, 116th Street, New York, New York 10027.

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complete an evaluation of the molecular modeling computer experience at the end of the semester. The evaluation was used to determine their opinions about the experience regarding aspects such as: effectiveness, integration with course content, interest, benefit, what was liked best and least, advantages, and time commitment. Also students' opinions were elicited regarding the helpfulness of the molecular modeling computer experience for 3-D visualization of atomic and molecular structure and whether their understanding of atomic and molecular structure was enhanced. The Institute for Learning Technologies, Teachers College, Columbia University developed the original evaluation form used in the two-year pilot study. The evaluation form used for this study is a modification of the pilot study evaluation.

Molecular Modeling

According to Casanova (1993) and others (McCormick, 1987; Box, 1991; Sauers, 1991; Weber *et al.,* 1992; and Gotwals, 1995) molecular modeling involves the use of a graphics-intensive computer that can model and manipulate images in three dimensions. Until about eight years ago the complexity of the mathematics behind molecular modeling only allowed research chemists to utilize it as a computational tool to design novel compounds such as structures that function as drugs, catalysts, or polymers.

The use of molecular modeling as an educational tool in the undergraduate curriculum has really only been prevalent within the past eight years as suggested by a number of journal articles (Canales *et al.,* 1992; Jarret and Sin, 1990; Lipkowitz, 1984; Rosenfeld, 1991; Sauers, 1991; Simpson, 1989; Shusterman and Shusterman, 1997). It is evident from three articles in *Chemical and Engineering News* (September 16, 1996; May 12, 1997; May 26, 1997) that the use of the computer as a computational tool is here to stay. Also software companies are remaking what was once a research tool for industrial scientists and developing it into a tool that is accessible and understandable to undergraduates and even to secondary students (Gotwals, 1995). Articles have also been published (Boyd and Lipkowitz, 1982; Cox, 1982) that help explain the molecular mechanics calculations that are so necessary for molecular modeling.

What is lacking, though, is evaluation of the use of molecular modeling at the undergraduate level. A report by the National Science Foundation (Breslin, 1991) discusses the issues and needs which pertain to innovation in science, mathematics, and engineering education and stresses the importance of rigorous evaluation for curricular and pedagogical innovations. It is necessary to begin asking questions about how the use of molecular modeling influences students, the evaluation of which will provide information to instructors who can begin to re-educate themselves in both the science and the technology (Ege and Chapman, 1993).

Computers in Science

Relevant Studies or Findings

Berger *et al.* (1994) reviewed past and present research on the uses of technology in science education. Several studies discussed in the review are pertinent to this study. One of these by Mokros and Tinker (1987) investigated the impact of microcomputer-based labs on children's ability to interpret graphs. They found that the generation of real data using microcomputer-based laboratories facilitated visualization of science concepts. The data were gathered while the students moved in front of a motion sensor and observed their movement being plotted on a real-time graph.

Also, Salomon *et al.* (cited in Berger *et al.,* 1994) suggest three important points regarding the use of intelligent technologies and how these can extend human intelligence. First, computers "potentially allow a learner to function at a level that transcends the limitations of his or her cognitive system" (p. 473). Second, once people have used a technology they may develop "thinking skills and strategies that reorganize and enhance their performance even away from the technology in question" (p. 473). Learners may be able to approach new problems with cognitive skills they did not have previously. Last, learners need to be in a state of readiness and know that the technology will work.

Berger *et al.* (1994), regarding the future of technology in science education, reached several conclusions. Technology will truly empower students to learn. The use of technology will not replace the instructor but will support the instructor. Technology will provide a solution to a pedagogical goal of instruction because it will be able to reach "a diverse range of students with varying learning needs" (p. 487).

In a study by Collins (1991) a rationale is presented for adding technology in schools which supports a constructivist view whereby teachers are facilitators ‘‘who help students construct their own understandings and capabilities in carrying out challenging tasks’’ (p. 29). The trends that have been observed in schools that have adopted computers are: small group instruction, coaching students vs. lecturing, more engaged students, assessment based on products, progress and effort, cooperative social structure, different students learning different things, and integration of visual and verbal thinking.

Milner and Wildberger (1974) addressed the issue of how computers should be used in learning. They suggested the use of computer simulations of science experiments that otherwise might be difficult to do because of safety, lack of equipment, or cost. In the present study, students were presented with an opportunity to become acquainted with a molecular modeling program. Previously used only as a research tool, this application exposed them to real-world problems such as those utilized by pharmaceutical companies to simulate the synthesis of novel compounds. The authors proposed a continuum of instructional uses of computers that ranged from drill and practice to interactive information retrieval to student-developed simulations of real systems or processes to student-designed automation.

In a study by Mokros and Tinker (cited in Kozma, 1991) the microcomputer-based lab (MBL) was used with seventh and eighth graders for three months. Temperature probes were linked to the computer and students could observe the increase and decrease of temperature as it was instantaneously graphed over time. There was a significant increase in the students’ ability to interpret graphs and the students made the greatest gains on items where graphs were used as part of the question.

In a study by Brasell (cited in Kozma, 1991) who also used MBL, but for physics instruction, data were collected in real-time and the posttest scores for the MBL treatment group were significantly higher than for any of the other treatments. A connection between symbols and the real world was realized immediately by the MBL students due to the transformation capabilities of the computer.

Casanova and Casanova (1991) studied the effects on the organic chemistry lecture course when enhanced with a variety of graphics and simulations employing different software packages. Nearly all of the lecture material resided in the microcomputer. Because chemistry is symbolically based, the authors believed that the organic chemistry course would provide an opportunity to equip students with important cognitive abilities. These were ‘‘the ability to create three-dimensional mental images, the ability to visualize the way atoms bind together, and the ability of qualitative pattern recognition’’ (p. 31). The results of the intensive microcomputer based course at the end of the first quarter were that students took very few notes, there was unusually high class participation, and students felt they had a good understanding of the subject. They also had very poor performance, though, on the conventional examination at the end of the term. Advantage was taken of this and student evaluations and modifications were made in the second quarter so students became more actively involved in the course through graded homework and a written weekly lecture synopsis. Compared to a control section, performance by the experimental section students improved dramatically in the second term. Several conclusions were reached based on the study:

(a) The increased amount of information that can be presented may interfere with students’ ability to absorb the additional information.
(b) Graphic, pictorial, written, and spoken information can be presented simultaneously, however, the question arose. ‘‘Does this enhance learning or make assimilation, integration, and recall more difficult?’’ The additional homework assignments second quarter probably helped students to reconstruct and integrate the multiple concurrent stimuli and begin to process it.
(c) There was greater reliance on metaphor, illustrations, and imaging, but students at the introductory level need to be carefully guided to link chemical imagery with chemical theory. Providing undergraduate chemistry students with pictures and movements of models have profound implications since these were previously only envisioned and manipulated in the imagination (Casanova, 1996).
(d) A change in lecture format from words and theory to graphics and visualization requires a different type of test than the traditional paper and pencil algorithmic test usually administered.

Use of Molecular Modeling

Casanova (1993) presented a historical overview of computer-based molecular modeling in chemistry and attributed the development of molecular mechanics as the force behind introducing molecular modeling as a routine tool. Empirical force fields for molecular properties were first proposed and employed by Westheimer (1946) and later by Warshel (1968) and Boyd (1970), but Allinger (1971) had the greatest influence on its utilization for routine use in the classroom. Bartell (1968) discussed one the first uses of computational molecular models in the classroom pertaining to the bonded and non-bonded distances of atoms in a molecule as it related to the valence shell electron pair repulsion theory.

An article in 1982 by Cox described the applications of molecular mechanics calculations and how they are used to investigate molecular conformations, thermodynamic properties, and vibrational spectra. Boyd and Lipkowitz (1982) spoke at the Quantum Chemistry Program Exchange Workshops on Practical Applications of Quantum Chemical Methods where they found that a large majority of industrial scientists routinely used molecular mechanics, but few academic scientists were familiar with it. They discussed the philosophy of molecular mechanics and recommended that teachers of chemistry let their students do their own molecular mechanics calculations and that even freshman chemistry students could do their own calculations.

Lipkowitz (1984) involved his organic chemistry lab students in the theory behind molecular mechanics and then, through the purchase of computer models from the Quantum Chemistry Program Exchange, had them compare computer models with physical models of the same structures. He recommends that students understand that physical models are limited in scope and can give misleading structural information. Also it should be stressed that the computer program is not a black box, that there are limitations to the data collected, and without an explanation of the theory, there is little intellectual involvement for the students.

In 1989 Simpson introduced organic chemistry students to molecular mechanics through several exercises in which molecular structures were optimized energetically and the results printed for the students to observe. The idea was that this would supplement physical models and the students would have to think about structures in three dimensions. Also, they would become acquainted with a technique that has many research applications and they would learn skills that would be applicable in higher-level laboratory courses.

Jarret and Sin (1990) also used molecular modeling with organic chemistry students and suggested a combination of both computer and physical models. Where physical models are useful for 3D visualization, they do not help students understand intramolecular and spatial relationships. Students had to first construct a physical model or draw the molecule in order to enter data in the computer about the location of each atom. The author suggested that the combination of molecular and physical models presented a more complete approach to the instruction of stereochemistry.

Two studies, both done in 1991, one by Sauers and the other by Rosenfeld incorporated molecular modeling into organic chemistry. Sauers indicated that his exercises had pedagogical value because students had to select their own structures, two isomers, and had to rationalize the difference in steric energies. This required them to question the conformation of molecules that would be strained. Upon completion of the exercise they had to discuss the output for their pair of structures. He concluded that it gave the students an appreciation for molecular modeling and real experience in computational chemistry. Rosenfeld's students, after completion of a tutorial, received a problem set with five or six questions, i.e., a comparison of strain energy and bond angles for several compounds. He indicated that he wanted his students to understand that molecular modeling is a tool for understanding chemistry and aids in problem solving in much the same way physical models are used.

Box (1991) described a molecular graphics program he wrote that enabled the organic chemistry student to construct, modify, examine, and manipulate organic chemical structures on-screen. Though he does not describe an experience in which it was used with students, he does go into detail regarding the use of computer-assisted molecular modeling for a specific structure.

Canales *et al.* (1992) described the use of molecular modeling in an undergraduate junior/senior level inorganic analysis and synthesis class. The exercise their students did introduced them to molecular mechanics and by modification of various aspects of molecules, the students gained an understanding of the theory behind molecular mechanics. A number of applications for molecular modeling are presented by Weber *et al.* (1992) as well as detailed descriptions of various options available for viewing structures.

DeKock *et al.* (1993) presented an excellent chapter on computational chemistry in the undergraduate curriculum. They presented background information on its use, curriculum issues related to computers and quantum chemistry, quantum chemistry, molecular mechanics, and molecular dynamics. They also reviewed molecular mechanics in the classroom and then described in a fair amount of detail the integration of computational chemistry at four universities. There were several important aspects they considered important concerning the use of computational chemistry:

(a) Students should emerge with the ability to create three-dimensional mental images, something that in Western civilization has not been important for several centuries.
(b) The use of the computer as a computational tool needs to be presented in the context of a particular chemical problem.
(c) Just as students are supervised in traditional experimental laboratories, there needs to be supervision in computational laboratories to prevent student frustration.

Hanks (1994) utilized a specific molecule and took the reader through different models of that molecule such as easy to draw pen and paper structures, ball and stick and space-filling computer generated representations, potential energy map, electron density cross section, electron density isosurface, and electrostatic isosurface. He discussed the importance of helping students develop models of the microscopic universe and that computer generated models not only deliver the message that molecules are three-dimensional, but quantitative information can be provided by the computer.

Gotwals (1995) introduced high school students to computational chemistry. He wanted them to be able to represent the dynamical nature of chemical systems through manipulation of the conditions of a system and then interpret how the dynamics of the system changed. Computational science would then be coupled with scientific visualization. Through national, corporate, and university sponsorship his students entered a national scientific problem-solving competition and had access to state of the art scientific workstation computers at their school while completing their competitive projects. The competition afforded him and his students the opportunities to successfully introduce computational chemistry at the high school level.

Shusterman and Shusterman (1997) utilize molecular modeling in their general and organic chemistry courses, respectively. They have written an excellent article about teaching chemistry with electron density models, the philosophy behind why this is pedagogically important, and the chemistry. The article is complete with diagrams that illustrate the salient points. Since electronic structure affects molecular size, shape, bonding, stability, and reactivity, the introduction of computer-generated electron density models will help students begin to have a better understanding of the role that electron structure plays in chemical phenomena.

Martin (1998) has introduced molecular modeling into the undergraduate curriculum starting in Organic Chemistry laboratory and then proceeding through senior level courses in Advanced Organic Chemistry and Physical Chemistry. In the Organic Chemistry course students learn the theory behind molecular modeling, complete exercises in which they learn how to perform various operations, and then combine what they have learned with a laboratory exercise. The success of this integrated approach has been measured through moderate increases in tested competency in selected aspects of three-dimensional chemistry and also rapid increase in enrollment in upper-level chemistry courses and an increase in the number of majors and minors.

METHOD

Experimental Design

The treatment consisted of the use of a molecular modeling computer program Spartan (Wavefunction, Inc., Irvine, California) where students were able to build, manipulate, measure, rotate, and change the size of models of atomic and molecular structures. The computer experience took place in a computer laboratory utilizing a UNIX-based platform with Silicon Graphics Indigo series workstations. Students visited the computer laboratory four times during the semester for two-hour sessions to complete exercises on the atomic and molecular structure of various species. The students were exposed to a pre-lecture one week before beginning an exercise which served to focus their attention on difficulties that might arise in utilizing the computer program, the questions in the exercises they were required to complete, and on various aspects of atomic and molecular structure.

The sample from which the treatment group was randomly chosen consisted of approximately 600 students enrolled in the first semester chemistry course. Though the students were registered for two different sections with two different professors, both professors lectured to all students for one or more units. One professor lectured for two-thirds of the semester and the other professor for one-third of the semester. This served to minimize any differences between the two professors. The treatment group who used the molecular modeling computer program consisted of 129 students.

Students in both the treatment and non-treatment groups met for three credit hours per semester, i.e., two times per week for one hour and fifteen minutes for the course lectures. Three Fridays of the term were utilized for multiple-choice exams. On three different Fridays of the term students in the treatment group attended a lecture demonstration regarding the molecular modeling computer program. These were designed to better integrate the course content with the computer experience, explain chemistry concepts, and show the students how to utilize various aspects of Spartan.

To minimize differences in the treatment and non-treatment groups in terms of the time commitment of the treatment group in the computer lab and exercises they were required to complete, each student in the non-treatment group was required to read one book during the semester from a suggested reading list. They were required to submit a thesis statement and an abstract to their chemistry recitation teaching assistant that resolved some problem the author was trying to solve. They also attended two Friday lectures pertaining to the books on the reading list. The writing assignment counted the same number of points toward the final grade of the semester as the computer exercises. A variable that possibly confounded the study was the time required of the treatment group in the computer room and to complete the exercises. On an evaluation form that the treatment group completed, about 2% of the treatment group indicated that an advantage to doing ChemGate was that they did not have to do the writing assignment. About 2% also indicated that a disadvantage to ChemGate was that it was more work to do than the writing assignment, so the time variable was possibly not that much of an issue.

Students from both groups were also enrolled in a weekly recitation section taught by a graduate teaching assistant in the chemistry department. The recitation section met for fifty minutes each week. All students were allowed to specify their first and second choices for their recitation section without knowledge of the teaching assistant for a section. Placement in the various sections was done based on approximate size limitations.

The first of the four computer sessions was devoted to using a tutorial in order to become acquainted with various aspects of the molecular modeling program plus students had to answer questions pertaining to periodic trends of atom and orbital size. They learned to build structures, make measurements (bond angle and bond length), rotate and translate, change the scale of the models, and view and interpret a model's charge distribution.

For the remaining three sessions, the students completed exercises utilizing structures that had been prepared for them which were found in a directory they could access while using Spartan. Comments from the two-year pilot study indicated that the exercises had not been well integrated with the lecture course, therefore efforts were made so that the exercises for this study were integrated more closely with the lecture course and the order in which the material was presented in lecture. The majority of each of the exercises required that the students be present in the computer lab in order to view structures, manipulate models, and make measurements. It was necessary that students complete some questions outside the computer lab. The questions required students to synthesize the observations and measurements they made while in the computer lab. Selected reference materials were suggested that assisted the students in answering the questions. The general topics for the four exercises were: Exercise I, Trends in the Periodic Table; Exercise II, The Structure of Molecules; Exercise III, The Electronic Structure of Molecules; and Exercise IV, Properties of Organic Molecules.

On the evaluation form for the closed (multiple response items) response choices, a tally was done for each question and the percentage calculated for each choice. Tables were designed which organized this information. All open response choices on the evaluation form to a particular question were transcribed together and categories of similar responses were determined. A code was set for each category. All responses were then coded. Students could have more than one code for their response to a particular question. An expert with thirty years of teaching Advanced Placement Chemistry as well four years as an instructor in first year college chemistry was trained in the coding process. A sample of ten percent of all open response questions was randomly chosen which the expert coded. There was an agreement of 90% between the author and the expert.

RESULTS AND DISCUSSION

The results of the closed response choices on the Evaluation completed by the treatment group at the end of the semester are shown in Table I. Specifically used were a Likert scale set of questions and open-ended response questions. As shown in Table I approximately 72% of the students agreed or strongly agreed that computer-based resources were effective for learning Chemistry. They indicated (55% or greater) that the exercises completed during the computer experience were supportive and helpful for the content covered in chemistry lecture with the Professor or for content covered in the textbook for the class. Sixty-five percent of the students felt they benefited from having used computer-based resources.

Sixty-four percent felt there would be a future benefit to having used computer technology. I wanted to know whether students who had participated in the pilot study the previous year would feel they had benefited from the use of molecular modeling in their present science courses. Unsolicited comments from five students who were in Organic Chemistry and/or Biology during this study were obtained at the end of the year of the aforementioned courses. Their comments were the following:

Table I. Results of the ChemGate Evaluation[a]

	5[b]	4	3	2	1	No response
1. Computer-based resources used in this course were effective for learning Chemistry.	16.5	55.4	19.8	5.0	2.5	0.8
2. I developed a stronger grasp of relevant chemistry concepts by using computer-based tools.	19.0	50.4	19.0	7.5	3.3	0.8
3. The computer work and the non-computer work in this course were well-integrated.	6.6	38.9	23.1	27.3	4.1	
4. Overall, I feel I benefited from the fact that chemistry recitation used computer-based resources.	16.5	48.8	20.7	11.5	1.7	0.8
5. Chemistry is interesting to me.	12.4	48.8	31.4	3.3	4.1	
6. I feel that there will be a future benefit to my having used computer technology.	24.8	39.7	24.0	10.7	0.8	
7. I found the ChemGate exercises helpful for 3-D visualization of molecular structure.	42.9	47.1	5.8	1.7	1.7	0.8
8. I worked cooperatively on problem solving with students on ChemGate exercises:						
a. During ChemGate recitation.	13.2	34.6	19.9	19.9	12.4	
b. At times other than ChemGate recitation.	14.9	38.0	14.0	14.9	18.2	
9. I used additional support to complete the ChemGate exercises:						
a. Textbook for the class.	24.8	52.1	11.6	4.9	6.6	
b. Other books.	2.5	8.3	13.2	24.0	51.2	0.8
c. Instructor in the ChemGate recitation.	13.2	34.7	17.4	18.2	16.5	
d. TAs in the ChemGate recitation	25.6	43.9	13.2	7.4	9.9	
e. TAs other than ChemGateTAs.	3.3	6.6	19.0	26.4	44.7	
f. Professor for the lecture aspect of the course.	2.5	13.2	19.8	24.8	39.7	
g. Other people or sources.	7.4	22.3	19.9	18.2	32.2	
10. I found the ChemGate exercises to be supportive and helpful for the:						
a. Content covered in regular recitation.	5.8	31.4	37.2	17.4	7.4	0.8
b. Content covered in chemistry lecture with the Professor.	6.6	48.8	28.9	10.7	5.0	
c. Content covered in the textbook for the class.	10.7	50.4	28.1	8.3	2.5	
11. I would like to have seen better integration of ChemGate recitation and Chemistry lecture.	38.0	34.7	18.2	8.3	0.8	
12. I utilize models (mental or written) when:						
a. I am studying the textbook for the class.	18.2	48.8	23.1	7.4	2.5	
b. I am studying my notes for the class.	14.9	36.4	27.3	15.7	5.7	
c. The Chemistry Professor lectures.	15.7	35.5	30.6	12.4	5.8	
d. I am in other classes besides science.	11.6	25.6	26.4	19.9	16.5	
13. I feel my understanding of atomic and/or molecular structure was enhanced by ChemGate recitation.	27.3	47.9	16.5	5.0	2.5	0.8

[a]All values are recorded as percentages.
[b]5 = strongly agree; 4 = agree; 3 = neutral or undecided; 2 = disagree; 1 = strongly disagree.

(a) It was a very effective learning tool for Organic I and II because it helped make SN2 reactions easier to understand. It made the use of molecular physical models easier to use because of having visualized the shapes of molecules on the screen. It helped with bond lengths, bond angles, chirality, enantiomers, and diastereomers. Also the graphical representation of the potential energy curve for different conformations made it easier to understand the varying energies of conformers.
(b) It helped both at the very beginning and end of Organic because it allowed the stereochemistry to be more understandable and not brand new. It helped in Biology with protein structure and amino acids.
(c) While time consuming it did help me in Organic. I didn't have to see things for the first time. I'd seen primary, secondary, and tertiary structures of peptides and an SN2 reaction. I'd drawn chemical structures. I hated it as a general student, but I liked not being so surprised as others in Organic.
(d) It was useful for visualizing shapes of molecules—otherwise it was more helpful in Biology for understanding protein structure.
(e) Many of the visual/spatial concepts of Organic were illustrated with the computer experience (protein structure, energy barriers and rotation around a single bond). I felt I was better prepared for Organic having done it, though it didn't fit with General Chemistry.

After the fact, though time-consuming and perhaps difficult, students one year later do indicate they benefited from the experience.

Students were asked what they liked best about the experience and what were the greatest advantages. The responses for these two questions are grouped together in Table II. A student's response could be coded in more than one way. For example, one student indicated that, "It provided a chance to do visualization and enabled us to look at Chemistry in a different way. It nicely complemented the book and lectures." This student's response was coded under visualization, understanding, and fun/interesting.

The most important advantage of ChemGate was the visualization aspect of the three-dimensional nature of models and the structure of molecules with 86.8% of the students indicating this advantage.

Table II. The Responses for the Following Two Questions Were Combined: 14. The Things I Liked Best About ChemGate Recitation; 16. What, in Your Opinion, Were the Greatest Advantages of Learning Chemistry with Computer-Based Resources?

Categories	Percentage[a]
Visualization—3-D models, structure of molecules	86.8
Understanding—focus on textbook material, learn, extend understanding, abstract ideas more concrete	38.8
Computer usage—liked it, fun, easy to use, Spartan	37.2
TAs—helpfulness, there to answer questions	11.6
Integration—ChemGate with lecture	10.7
Fun, interesting	8.26
Hands on experience	5.79
Time—number of meetings, brevity	3.30
Chemwrite—did not have to do it	2.48
Exercises—in-class	1.65
None—no disadvantages	0.83
No response to the questions	4.13
Negative response	1.65

[a]Percentages do not total to 100%. They represent the number of different students whose response was coded under the category.

Thirty-eight percent felt that it helped them focus on textbook material, extend their understanding, and make abstract ideas more concrete. They also felt (37.2%) that the computer was fun, easy to use, and that they liked it and the computer program, Spartan. On one section of the Likert scale questions, 61% of the students agreed or strongly agreed that Chemistry was interesting to them. In a study by Culp and Lagowski (1971) students completed a Likert scale pertaining to student attitude. Students responded favorably "regarding the time required for participation (in computer-assisted instruction), assistance in learning the material, continuation of the program, and general enjoyment" (p. 361).

Table III indicates the disadvantages of the computer experience and aspects the students liked least. Again a student's response could be coded in more than one category. For example one student indicated that the "Programs weren't very practical. Essentially felt like looking in a dictionary, since all values were pre-calculated for the program." This response was coded under the categories computer and tedious. The disadvantage that received the highest percent, 27%, was an expression of a dislike for the computers, themselves, that they could learn better without them, and that there were shortcomings to Spartan applications. Twenty-seven percent also felt there was a time problem that included poor scheduling, too much time required so they had to complete the

Table III. The Responses for the Following Two Questions Were Combined: 15. The Things I Liked Least About ChemGate Recitation; 16. What, in Your Opinion, Were the Greatest Disadvantages of Learning Chemistry with Computer-Based Resources?

Categories	Percentage[a]
Computer—how it was used, hate them, not enough of them, learn better without, values pre-calculated, shortcomings of Spartan	27.3
Time—scheduled poorly, too much time required, couldn't complete during class	26.4
Lack of integration—ChemGate with lecture	22.3
Exercises—unclear directions, difficult, more detail needed	19.8
Tedious—measurements repeated, boring, no thinking to measurements, pointless questions	18.2
TAs—not interested, could not explain, did not help	12.4
Understanding—doesn't explain theories	11.6
Grading—not graded soon enough	3.31
Register—didn't know at registration	3.31
Chemwrite—more work to do than it	0.83
Interaction—lack of interaction with others	0.83
Lab—not open at other times	0.83
None—no disadvantages	15.7
Positive responses	6.61
No response to the questions	11.6

[a]Percentages do not total to 100%. They represent the number of different students whose response was coded under the category.

Table IV. 17. If You Indicated Earlier that the ChemGate Exercises Were Helpful for 3-D Visualization of Atomic and/or Molecular Structure, Please Elaborate on Your Choice. Also, if Visualization Is Not Something You Do, Please Explain

Category	Percentage[a]
Concept—polarity, molecular orbitals, dipole, hybridization, electron repulsion, electronegativity, VSEPR, atomic size, atomic shape, electron density, resonance	34.7
Geometry—orientation, interatomic relationships, shape, what it looks like, observe from all angles, different views, different atomic arrangements	23.1
Understanding—theoretical/abstract, grasp concepts	18.2
Rotate	15.7
Visual learner	9.1
1-D—one dimensional representations like a textbook	8.3
Organic chemistry—staggered vs. eclipsed	6.6
Image—picture in head	5.8
Molecular structure	3.3
Measure—bond length, bond angle	2.5
Zoom	1.7
Negative responses	0.8
No response to the question	13.2
Uncoded responses	4.1

[a]Percentages do not total to 100%. They represent the number of different students whose response was coded under the category.

exercises outside of class, and the lab was not open at other times. Also, 22% indicated that lecture was not integrated with the computer experience. This seems to be a problem no matter what care is taken to integrate the lecture with the computer experience. The semester in which these data were collected was the fifth semester in which computers were used and each term additional effort was made to integrate the use of computers with the lecture for the course. It is good to note that twice this percentage of students in the Fall of 1996 (the second year of the pilot study) indicated lack of integration, so better integration did occur during this study.

Tables IV and V pertain to students' responses on the helpfulness of the ChemGate exercises for 3-D visualization and understanding of atomic and/or molecular structure. On the Likert scale of the Evaluation (Table I) the percentage of students who agreed or strongly agreed regarding the helpfulness of 3-D visualization of molecular structure and that their understanding of atomic and/or molecular structure was enhanced were 90.0% and 75.2%, respectively. On the open response questions on the Evaluation 34.7% indicated that 3-D visualization was helpful with concepts such as polarity, molecular orbitals, dipole, and resonance, with 28.1% indicating that their understanding of these same concepts at the atomic and/or molecular level was enhanced. Approximately 26% indicated that visualization was helpful for orientation, shape, and molecular structure and 10.7% indicated their understanding of geometry at the atomic and/or molecular level was enhanced. Eighteen percent of the students indicated that visualization was helpful in understanding theory and grasping concepts.

The treatment group worked with a molecular modeling program, Spartan, that exposed them to the three-dimensional visualization of structures at the molecular level. As they worked at the computer, they also completed exercises that required them to combine what was being observed visually with chemistry concepts. They visualized:

(a) the manipulation of structures through zooming, translation, and rotation.
(b) the measurements of bond length and bond angle.
(c) electrostatic potential surfaces that further emphasized the negative and positive areas

Table V. 18. If You Indicated That Your Understanding of Atomic and/or Molecular Structure Was Enhanced by ChemGate, Please Explain How It Was Enhanced

Category	Percentage[a]
Concept	28.1
Visualization	25.6
Geometry	10.7
1-D—one dimensional representations as in a textbook	5.8
Manipulate—zoom, rotate, translate	5.0
Exercises—by answering the questions	3.3
Apply—application of the information	2.5
Attention—focus in on details	1.7
Image	1.7
Lecture	1.7
Measurement	1.7
TAs	0.8
Visual learner	0.8
No response	23.1
Same response as #17	9.1
Negative	1.7

[a]Percentages do not total to 100%. They represent the number of different students whose response was coded under the category.

on the molecules through a gradated color code (red more negative and blue more positive).

(d) the bonding and anti-bonding molecular orbitals of several species.

(e) periodic trends of different species.

Students mentioned the above as important in enhancing their understanding at the atomic and/or molecular level. It was evident from the results on the Final semester exam that students' understanding was enhanced and perhaps that can be attributed to the visualization of atomic and/or molecular structures in a number of different situations. They scored significantly better ($p = 0.0067$) on questions related to dipole moment, resonance, and a chemical reaction question that required them to focus on the number of particles and their combination to form molecular and atomic species.

Other studies support the importance and relationship of visualization and understanding concepts. Baker and Talley (1972) found that visualization skills enhanced the ability of students to cope with concepts in chemistry. In another study by Talley (1973) students constructed models for each chemical species and its chemical interactions that were discussed in class. The idea was that concrete manipulation of the models would afford students the opportunity to visualize transformations taking place in chemical reactions. The study indicated that the ability to visualize in three dimensions resulted in transference of abilities to perform at higher cognitive levels such as application, analysis, and evaluation. Holliday (1975) found that students who used both textbook like pictures and verbal statements could process both instructional components leading to coherent meaningful integration of stimuli. Anderson (1972) has identified the powerfulness of the image-invoking qualities of a stimulus as an aid in the semantic encoding process (cited in Holliday, 1975 p. 78).

Table VI contains students' responses concerning whether they would choose the computer-based chemistry section again. Seventy-six percent indicated they would. This was a 20% improvement from the evaluations received one year earlier in the Fall of 1996. Reasons given were various such as fun, educational, interesting, computer exposure, hands on experience, visualization, and a better understanding of chemistry. Only 12% indicated they would not choose the section again with reasons such as it took up too much time, it was not clear what was expected, it was difficult to get help, and there was lack of integration with lecture. The amount of time students spent on the exercises outside of regularly scheduled hours is shown in Table VII. This ranged from one to approximately two additional hours. Even considering the additional time spent on the exercises outside of class, the majority of students would still choose the computer-based chemistry section.

Authors who have used molecular modeling in their courses have various anecdotal comments concerning its use. These comments are supported by the data from the Evaluation form of the students. Comments such as:

(a) Thinking about structures in three dimensions is an important skill for understanding organic chemistry. They become knowledgeable about a technique that has many applications in research. Students will learn skills useful in higher-level chemistry courses (Simpson, 1989).

(b) Students begin to ask sophisticated questions related to molecular shape. The exercise was enlightening for students and invigorating for faculty (Lipkowitz, 1984).

(c) Students benefit from a first-hand contact with molecular shape, as well as with computers (Boyd and Lipkowitz, 1982).

(d) "Graphical models help students synthesize different perspectives of a molecule, enhancing their understanding of structure and reactivity" (Hanks, p. 66, 1994).

Table VI. 20. If You Could Choose Again, Would You Choose the Chemistry Section that Used Computer-Based Resources? Why or Why Not?

Response	Percentage
Yes	76.0
No	12.4
Conditional	0.8
Undecided	4.1
No response	5.8

Response	
Yes	*No*
Fun enjoyable, educational, interesting	Took up too much time
Integration, relevance to lecture	Should have been incorporated into the daily lecture
Exposure to computers	Was not clear what was expected
Better understanding of chemistry	Difficult to get help from the TAs
Molecular explanation	Grading of the exercises not fast enough
Visualization	Chemwrite was more interesting
Hands on experience	Computer program not useful in the future
Spacing of class times was good	Lack of integration with lecture
Theory/abstract/concepts—interactive, reinforce	Needed other resources besides the textbook
Help with organic chemistry	Too much work
Chemwrite not as interesting	
Geometry of the molecules	
TAs helping students	

(e) Modification of the force field allows student to see parameters that will hopefully give them an appreciation of their function (Canales, Egan and Zimmer, 1992).
(f) Students have been quite enthusiastic and anxious to help each other over the practical problems associated with the calculations (Rosenfeld, 1991).
(g) Students gain an appreciation of the interplay of molecular forces. The project was well received by most students involved, they felt it was interesting and challenging, and it provided them with a real experience in computational chemistry (Sauers, 1991).
(h) An experience of this type introduces students to the use of computers in science and should make them more comfortable with more advanced applications (Jarret and Sin, 1990).

Table VII. 19. Other than the Time Required ChemGate Recitation Hours, Approximately How Much Additional Time Outside of ChemGate recitation Did You Spend on Exercises 2, 3, and 4? $N = 114$

	Exercise		
	II	III	IV
Mean	1.1	1.2	1.7
Standard deviation	0.85	0.97	1.1

CONCLUSION

Molecular modeling provides an opportunity to enhance the visual analysis of students. Neisser (1997) indicated that children exposed to extensive visual media develop specific skills of visual analysis. It is important to keep this in mind when writing curricula to accompany a molecular modeling experience. Organic chemistry students, one year later, indicated that the experience gave them a ‘‘head start’’, but the conceptual level of the students needs to be kept in mind. Also, what are the capabilities of the students in terms of computer skills? Is there a well written tutorial on the needed computer commands that will provide a solid basis to get them started and which will reduce unneeded frustration about the computer and the computer applications? Is the tutorial that accompanies the software adequate for the students who will be using it, or should it be rewritten so it will serve the needs of the students? What scientific understanding and knowledge do the students bring with them to the experience? Has this been addressed before students begin exercises that require them to integrate multiple concepts?

Molecular modeling has been an untapped resource until approximately eight years ago when it was first integrated into the undergraduate curriculum in organic chemistry. This study investigated the assessment of the first major integration of molecular modeling computer applications into an introductory course, where for some students, chemistry will be their terminal course. A project of this nature can be used to assist others in accomplishing similar goals. What has been learned is that it can not be done without teamwork, continuous formative evaluation, monetary support for computers and a support staff of teaching assistants, and a time investment that exceeds what would be considered ''normal''. There needs to be a re-evaluation of the computer experience each semester molecular modeling is utilized addressing such questions as: What did work? What did not work? What can we do better? Most of all, what did the students have to say about the experience? Can we make immediate changes that address their evaluative opinions? What long-term changes can be made that will make the experience more meaningful and better for students? We are only at the beginning of the evaluative process of the present and potential effect of molecular modeling into introductory courses. This study has provided a beginning for others who are interested in investigating the effects of a unique aspect of computer technology on students' learning.

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