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ABSTRACT

The Water and Molecular Networks (WAMNet) Project uses graduate student written Reduced Instruction Set Computing (RISC) computer simulations of the molecular structure of water to assist high school students learn about the nature of water. This study examined: (1) preconceptions concerning the molecular structure of water common among high school students; (2) the effect of making and testing predictions using visual, interactive computer simulations on students' conceptions of the microscopic properties of water; and (3) aspects of the simulations that were most helpful in promoting conceptual change. Ten students from high schools in the Boston, Massachusetts area participated in 50 hours of individual and pair demonstration interviews in which students were asked to think aloud and interpret what they saw on the computer screen as they used the computer simulations. Analysis of transcriptions of the interviews indicated that: (1) students had preconceptions concerning the composition of individual water molecules and the structure of molecular water in ice, vapor, and vapor forms; (2) student concepts of water composition, the molecular structure, and the relationship between the kinetic energy of particles and their temperature changed as a result of working with the water simulation; and (3) visualization, multiple representations, interactive control of parameters, and debate with partners contributed to that change in the students' concepts. Contains 14 references. (MDH)

THE EFFECT OF INTERACTIVE, THREE DIMENSIONAL, HIGH SPEED SIMULATIONS ON HIGH SCHOOL SCIENCE STUDENTS' CONCEPTIONS OF THE MOLECULAR STRUCTURE OF WATER

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The effect of interactive, three dimensional, high speed simulations on high school science students' conceptions of the molecular structure of water†

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OBJECTIVES

The primary objectives of this study are to (1) document preconceptions concerning the microscopic and macroscopic properties of water held by high school science students and (2) determine whether interactive, visual, computer simulations designed specifically to address these preconceptions improve student understanding of the structure and properties of molecular water.

INTRODUCTION

Several researchers have examined what students believe about the macroscopic and microscopic properties of water. For example, Giese (1987) constructed and analyzed a written test on water pressure and found that middle school students in her investigation held numerous preconceptions. Novick and Nussbaum (1981) have studied student understanding of the particulate nature of matter. Griffiths and Preston (1992) recently published one of the most extensive studies of student preconceptions concerning water molecules. In their investigation, thirty high school students were interviewed extensively. Griffiths and Preston found that students held significant preconceptions concerning the structure, composition, size, shape, bonding, and energy of water molecules. Furthermore, Griffiths and Preston reported few differences between the preconceptions held by students with strong science backgrounds and their cohorts who had received little or no formal instruction.

Griffiths and Preston suggest three possible reasons why students hold preconceptions about water molecules. First, scientific models of molecules are typically presented in a way that make them appear abstract and unrelated to everyday experience. Second, the particle nature of matter is so innately

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complex and difficult to visualize that students are forced to construct cre ive and unorthodox conceptualizations. Third, in an attempt to help students visualize the sub microscopic world, textbooks often present contradictory models of atoms and molecules. Such inconsistencies may lead to additional confusion.

A possible way to improve student understanding of the molecular structure of matter is to use currently available computing power to develop visual, dynamic, and interactive simulations for the science classroom. Computer simulations that address student preconceptions concerning molecular water are being developed by undergraduate and graduate student programmers at Boston University. These visual, highly interactive simulations employ the speed of RISC-based (Reduced Instruction Set Computing) workstations to model the three-dimensional structure of molecules and the hydrogen bond network that holds water molecules together. By varying various macroscopic parameters (e.g. temperature and pressure), students can use these simulations to make and test predictions concerning the microscopic properties of water molecules.

RATIONALE

Research on student science conceptions has been an increasingly significant component of the educational literature over the past three decades (Wandersee and Mintzes, 1987). The increasing popularity of this kind of research has generally been attributed to the growing acceptance of the constructivist view of learning (Gunstone and Northfield, 1986). In constructivism, students are not viewed as "blank slates" who passively absorb what we teach. Instead, constructivism views learning as an interaction between new experiences and existing conceptions that occur within students rather than between students and teachers.

When a student's existing conception contradicts accepted scientific explanations, they are often called "misconceptions" (Fisher, 1983), "preconceptions" (Ausubel, Novak, and Hanesian, 1978), "alternative conceptions" (Hewson & Hewson, 1983), or "naive theories" (Resnick, 1983). While the terminology chosen to describe student beliefs varies widely and reflects sli y different philosophical perspectives, there is substantial evidence suggesting that student preconceptions are pervasive, interfere with science learning, and are highly resistant to change.

Student science preconceptions represent the following challenge for software developers: how to design simulations for science classrooms that address and eliminate student-held preconceptions? Several curriculum developers, science educators, and cognitive theorists have chosen to develop computer simulations based on the results of their own research on student concept development. These researchers have reported success in promoting the adoption of scientific conceptions when they took student preconceptions into account and made software sufficiently interactive (White and Horwitz, 1987; DiSessa, 1987; Pea and Sipusic, 1990; McDermott, 1990). Snir, Smith, and Grosslight (1988) call for the development of "conceptually enhanced" computer simulations which allow students to observe and experiment with what cannot be directly observed in the laboratory. Such simulation show the relationships between concepts. Snir et al believe that only with such simulations can educators truly address and change students' incorrect preconceptions. The designers of such simulations base the code of the program on the physical laws that underlie the system that is being modeled rather than simply programming a set of screen which will be viewed in sequence.

This paper describes results from ongoing research on student preconceptions concerning the molecular structure of water. We will also describe how the results of this research are being used to evaluate and modify the RISC-based computer simulations being developed for high school chemistry and physics students. Finally, we will present evidence from individual demonstration interviews that suggest that these simulations address and eliminate student preconceptions, even among disadvantaged inner-city students with little or no science backgrounds.

OVERVIEW OF WAMNET PROJECT

The setting

The Center for Polymer Studies at Boston University is composed of physics department faculty, post doctoral students, graduate students, and undergraduate students. Several years ago they decided to use their scientific expertise to bring current scientific research topics and methodologies to high school students. As the education project progressed graduate students who were studying the molecular structure of water adapted simulations that they had written for their own research into simulations that could be used by high school students to learn about the molecular nature of water. These simulations form the basis of the WAMNet (Water and Molecular Networks) project.

The purpose

The purposes of the WAMNet simulations are threefold. The first is to teach students how the macroscopic properties of water are related to its molecular nature. For example, students are told in science class that the higher the temperature of water, the faster the molecules are moving. With the computer simulation they can increase the temperature and see the molecules move faster. They can also use the computer simulations the hydrogen bond network and how the molecular structure of water evolves with changing thermodynamic parameters.

This leads to the second purpose, which is to give students visual models with which they can experiment. The aim is to help the students work as researchers. The questions that they research may not be completely novel to scientists, but they will be to the students. With the simulations, they can design the experiments themselves and thereby learn important research skills such as keeping the number of variables to a minimum, collecting data and analyzing data. This kind of research is difficult to conduct in the traditional high school chemistry laboratory because of the limited amount of equipment and inherent dangers associated with chemistry laboratories. A teacher cannot simply let students freely explore in the chemistry laboratory. With simulated experiments there are no dangerous chemicals or expensive equipment (with the obvious exception of the computer) needed. Computers are also not expendable and therefore do not need to be purchased every year.

The third purpose of the computer simulations is to teach students that models are not perfect; they have limitations. For example, the simulations cannot show the molecular structure of water as it freezes. The student can decrease the temperature below the freezing point but the program will not simulate the hexagonal lattice. The reason for this limitation is very simple. In order for the simulation to work properly it must take into account the vibrational motion of the individual water molecules. This means that the time step must be 10^{-15} seconds. The time scale for freezing water is on the order of 10^{-3} seconds. Therefore one could theoretically freeze water using the simulation, but it would take a very, very long time. This is one way students learn that models and simulations work within limited boundaries.

The simulations

The WAMNet programs are true computer simulations. They are not simply movies of computer screens but are driven by algorithms which represent the most current thinking about how molecules behave. They are the kind of "conceptually enhanced" computer simulations which Snir et al (1988) describe. Two simulations were used in this research, both of which were at preliminary stages of development. One of the simulations was used by each of the pairs for their first exposure to WAMNet. The molecules can either be represented as three dimensional "balls" with one large ball representing oxygen and two smaller balls representing hydrogen bonded to the oxygen or as "sticks" which look like boomerangs. Only one representation can appear on the screen at a time. This simulation allows the student a choice of two starting points: ice at $0^{o}C$ or water at $0^{o}C$. The second simulation was used by the pairs for four weeks, about two hours per week. The simulations presents the students with a container filled with 51 molecules of water. It uses the same two kinds of representations but allowed both to be seen on the screen at once. Only in the stick representation do the molecules actual move but the ball representation can be updated at any time to match the sticks. The student then has the ability to vary the temperature, pressure, and density of the container of water. With the three button mouse the student can zoom in or out of the container and can rotate the container in all three dimensions.

In addition the simulation allows for the insertion of an ion into the water. After choosing the charge of the ion a two dimensional potential energy landscape is drawn. This is color coded for the students to show them areas of high and low potential energy in much the same way that a color weather map shows area of high and low temperature. Students can move a grid around the container to see the potential energy landscape of any slice they choose. They then can choose the place where they think they will be able to insert the chosen ion. If the place they choose is acceptable, the computer will tell them so; if not it will ask them to choose another place. Once they have inserted the ion they can watch how the water molecules react to its presence and can see the formation of the hydration shell around the ion.

The student can experiment with all aspects of the simulation. All of the concepts in the simulation are concepts that are covered in many chemistry classrooms. They are not however ideas that are easily shown in traditional laboratory experiments.

RESEARCH QUESTIONS

This investigation addressed the following questions:

(1) What preconceptions concerning the molecular structure of water are common among high school science students?

(2) What effect does making and testing predictions using visual, highly interactive computer simulations have on student conceptions of the microscopic properties of water?

(3) What aspects of the simulations were most helpful in promoting conceptual change?

METHODOLOGY

Subjects

Ten students from high schools in the Boston area were interviewed in pairs and individually. The words and drawings of four of these students will be described in this paper. Here is a brief profile of these four students.

Kevin*: Kevin is a twelfth grade, African-American male from inner city Cambridge, MA. He had taken biology, and chemistry.

Mark: Mark is a twelfth grade, African-American male from inner city Chelsea, MA. He had taken biology, chemistry, and physics.

Diane: Diane is a ninth grade Hispanic female from inner city Boston. She had no science background and only basic math. Diane was very shy and very dismissive about her own abilities. She would start to say something and then say "never mind." Because of this there are not many quotes from her.

Mary: Mary a ninth grade Hispanic female from inner city Boston. She has no science background and only basic math.

* All of the students' names have been changed to maintain their anonymity.

Kevin and Mark worked on the simulations together. They were equally vocal. Mary and Diane worked on the simulations together. Mary was much more vocal than Diane.

Procedures

One of the purposes of the education project is to document some of the more commonly held preconceptions about the molecular nature of water and design computer simulations and other activities to confront these ideas. To that end the research group has done fifty hours of individual and pair demonstration interviews with ten high school students. In the demonstration interviews the students were asked to think aloud and interpret what they saw on the screen as they used the computer simulations. In the course of thinking aloud students voiced their preconceptions about water. The videotapes of these interviews have been transcribed and analyzed by members of the research team.

RESULTS

Preconceptions

From formal interviews and individual demonstration interviews the research teach uncovered preconceptions related to the molecular nature of water. Students had preconceptions about the structure of single water molecules, the molecular structure of the different phases of water, and how the molecules underwent phase changes.

Composition of individual water molecules:

On her first visit to the Polymer Center, Mary was asked to draw a water molecule. She was unable to do so. Mary told the researchers that she had learned that, "...water is H two O," but she did not know what, "...H and O means."

Unlike Mary, Mark and Kevin had well-developed ideas of what individual water molecules looked like. However, both students held profound misconceptions. Figures 1 and 2 are drawings done by Mark and Kevin before they worked with the simulations. Figure 1 shows a drawing collected from Mark. This student had successfully completed chemistry and physics yet he believed that a water molecule is composed of a mole of hydrogen and oxygen atoms held together by carbon bonds. The following is a portion of Mark's comments about the drawing.

> *Interviewer:* *What have you learned about water in school?*
> *Mark:* *It is made out of two elements. Oxygen and hydrogen -- and they have carbon -- that keeps them together.*
> *Interviewer:* *OK. Can you draw a picture of a water molecule? (Mark` draws).*
> *Mark:* *(Shows the completed diagram to the interviewer). I think it could look probably something like this (points at parts of the diagram with his pen). These things (indicating the 'sticks in the figure) would be carbon molecules that keep the molecules together and that (indicating the 'balls) would be a different molecule --*
> *Interviewer:* *OK, what are the circles?*
> *Mark:* *They are the other atoms.*
> *Interviewer:* *What kind of atoms did you draw?*
> *Mark:* *They are different ones. There are just two kinds, oxygen and hydrogen. They are linked by carbon.*
> *Interviewer:* *How many oxygen atoms and how many hydrogen atoms do you think the molecule has?*
> *Mark:* *I'm not sure? Moles or something.*

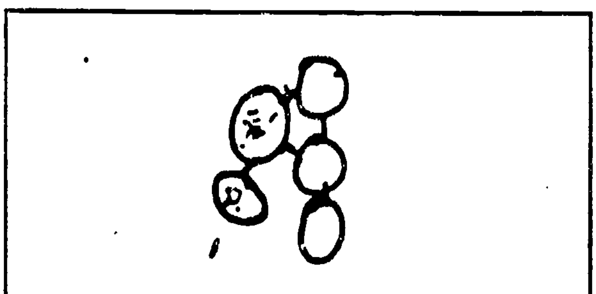

figure 1: Mark's first drawing of a water molecule

Kevin's drawing of an individual water molecule is shown in Figure 2. Unlike Mark, Kevin recognized that water is composed of one oxygen and two hydrogen atoms. however, when asked about "the stick" in his drawing, Kevin showed that his understanding was incomplete. The following are his comment about his diagram.

Interviewer: Can you draw me a picture of a water molecule?
Kevin: To draw!
Interviewer: It is just a guess, just what you think.
Kevin: (To himself) Two hydrogens and one oxygen... (To interviewer) May I use this (points at a paper)?
Interviewer: Yeah, go ahead.
Kevin: What do I think?
Interviewer: Yes. What do you think?
Kevin: (Picks up a pencil and speaks to himself) Two hydrogens and one oxygen...(Starts drawing) Two hydrogen... (To interviewer) Something like this? (Show drawing)
Interviewer: OK. What about those lines?
Kevin: I don't know. They seem, it looks like they are there. I don't know.

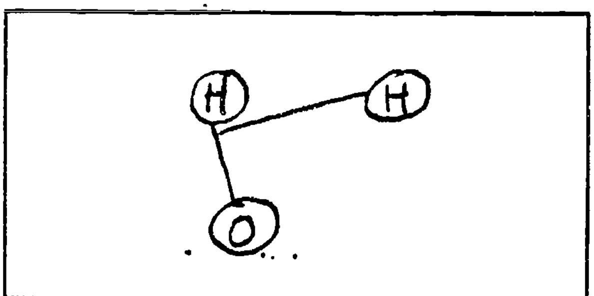

figure 2: Kevin's first drawing of a water molecule

Kevin has drawn a hydrogen bonded to the bond between a hydrogen and oxygen. Moreover, he could not articulate what the sticks in his figure represent and whether they really exist or not. It is important to note that we found these misconceptions among college student of all majors that we interviewed. Why do students who have taken or are taking chemistry and physics have so much trouble describing something as seemingly simple as a water molecule? Perhaps it is because they are taught a lot of vocabulary, but not given the tools needed to attach the appropriate concepts to those words. Many teachers, because of pressures of time and the need to "cover" the material, many teachers assume that their students understand what they have presented simply from words and perhaps a few static pictures. They do not have the time to really probe their students to determine if they have really understood.

Structure of molecular water (ice/liquid/vapor):

During the formal intake interviews, most of the students could not correctly draw the arrangement of water molecules in the solid, liquid, or gaseous states. Figures 3 and 4 show diagrams sketched by Mark and Kevin who were asked to draw how water molecules are assembled in ice, liquid water, and steam. Both students appear to hold the preconception that molecules of water are packed together more closely in ice than liquid. Here is a portion of Kevin's interview about his drawing.

> *Interviewer:* *And the balls are what?*
> *Kevin:* *The molecules.*
> *Interviewer:* *The molecules of water?*
> *Kevin:* *Yeah. ...in solid they are like...crunched up together...*
> *Interviewer:* *Hm.*
> *Kevin:* *(continues) ... in gas, they are separated - not separated, but ... not as close ... and liquid ... almost the same as gas, but still not too close together.*

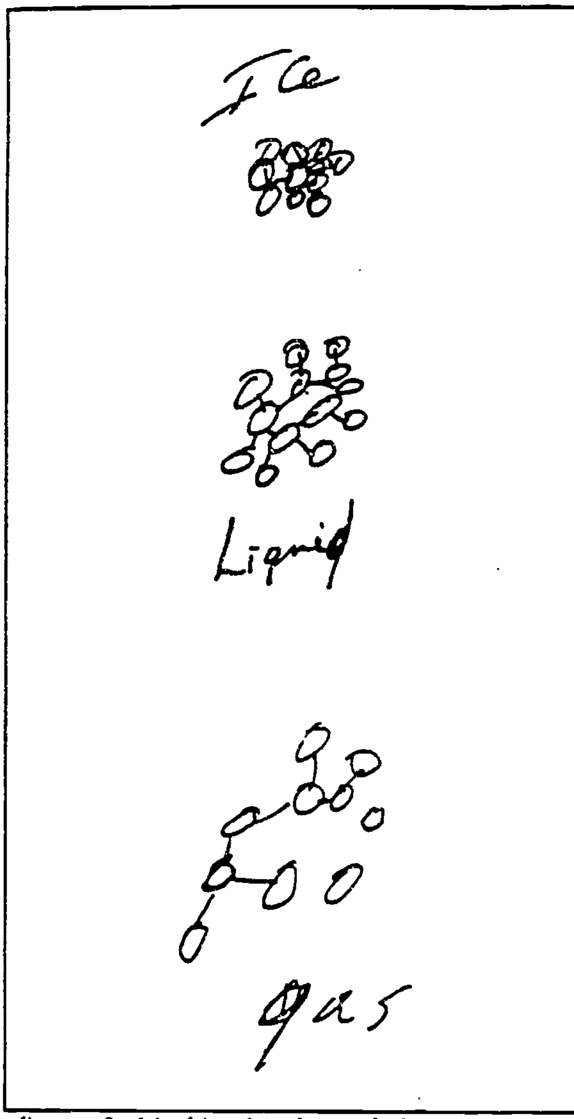

figure 3: Mark's sketches of the molecular structure of water in the solid (ice), liquid, and gas (steam) state.

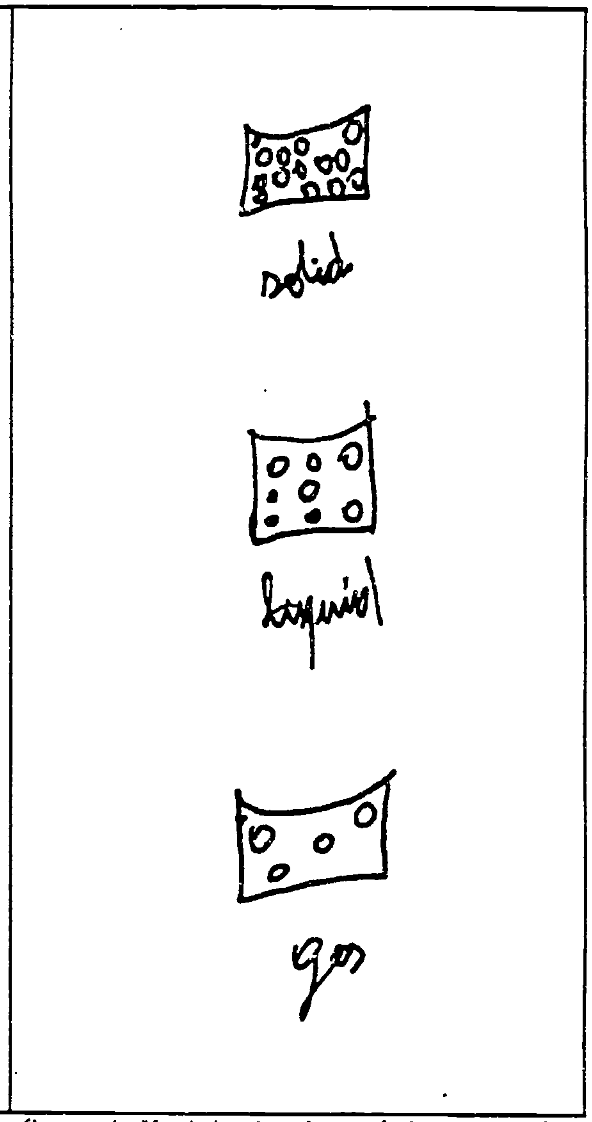

figure 4: Kevin's sketches of the molecular structure of water in the solid (ice) liquid and gas (steam) states.

Like Kevin, Mark also believes that water molecules in the solid state are more densely packed than in liquid or gas. Here is a portion of Mark's interview about his drawing.

> <u>Mark</u>: *They are close to each other when they are solid, they have a closer bonds between them, so the molecules don't move apart, which they would, it they were in another state. So, solids stay close to each other and - in liquid, they are kind of loose of each other, so the molecules are moving. And steam, or any other kind of vapor, is far apart and*

moving all over the place. Anyway, you don't see where they go.

Mark draws a picture of solid, liquid and gas.

.Mary held the same preconception regarding the density of ice, liquid, and gaseous water. In addition, Mary believed that water molecules break into free hydrogen and oxygen in the gaseous state.

> Mary: *When it's ice it's all of the molecules are stuck together and when it's water they are just loose, flying around. And when it's gas I think the hydrogen molecules break away from the oxygen molecules when it's a gas.*
>
> Interviewer: *So it's hydrogen and oxygen balls running around.*
>
> Mary: *Yes.*

The misconception that ice is more dense than liquid water may come from a common diagram in most physical science or chemistry text which shows the three states of matter with the molecules in the solid phase more densely packed than the liquid, and the liquid phase more densely packed than the gaseous. Kevin's diagram is similar to many such diagrams. The problem is that water is a special case, but that is not made clear enough to many students. The students simply remember the diagram.

As for Mary's idea that the atoms which make up a water molecule break apart in the gas phase, in a preliminary survey of 245 high school students conducted by the education project 45% of the respondents held Mary's misconception that hydrogen and oxygen break apart in the gaseous phase. Perhaps this is because the students are told that particles move far apart in the gas phase and they interpret this to mean that the molecule breaks apart. Again there is not enough time spent in school trying to probe and uncover what students really think and understand.

Conceptual change

Composition of individual water molecules:

What effect did the computer simulations have on student conceptions of water? The ideas of the three students described earlier underwent considerable change. After using the computer simulation they were able to explain that a water molecule consists of two hydrogens and one oxygen, draw the bond angle correctly, and describe the electrical polarity of the molecule and its significance. The following is Kevin's description of his diagram (figure 5). This discussion took place one week after Kevin and Mark explored the water simulations for the first time.

> *Interviewer:* *And to start off with, I just want you to do the same thing you did last week and ask you if you could draw what you think a water molecule looks like.*
> *Kevin:* *Aha! Well...I know it in my mind, but I am not sure if I can transmit it on the paper. A water molecule! OK. (Starts drawing.) One hydrogen actually, it is two hydrogens. I looks something like... Oh, yeah! (Draws, pause)*
> *Interviewer:* *OK. Great. So, what are the H's and O's?*
> *Kevin:* *H is a hydrogen and the O - the oxygen.*
> *Interviewer:* *It's two -*
> *Kevin:* *-hydrogens and one oxygen.*
> *Interviewer:* *So does every water molecule look like that?*
> *Kevin:* *Yeah.*
> *Interviewer:* *And what are the sticks?*
> *Kevin:* *Oh! Oh! They are not really sticks, I mean - it is just to show how ... [they connect] one to another.*

Kevin is clearly more confident in his answers and he has discarded his belief that the one hydrogen is bonded to the bond between the other hydrogen and the oxygen. He is also more confident that the sticks are not real.

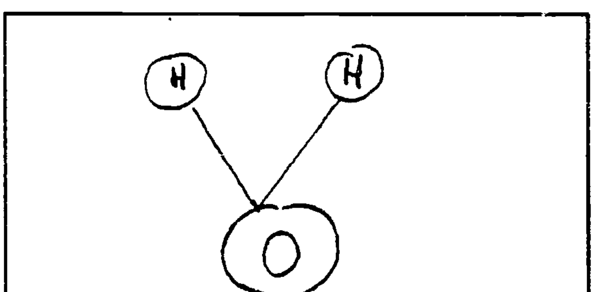

figure 5: Kevin's second drawing of a water molecule

Mark also made significant progress in his understanding of a water molecule after using the program for a few hours. In the following portion of an interview, Mark discusses his drawing (figure 6).

> *Interviewer:* *All right - what I thought I'd do today was - just start off by asking you pretty much the*

same question about water I asked you last week. Which is: can you draw a water molecule for me?
<u>Mark</u>: I'll try. (Picks up a pen and stars drawing.) ... Big ball... and a tiny little ball...(keeps on drawing...Something close to that... I still cannot draw.
<u>Interviewer:</u> No, that's pretty good. All right, tell me what those...what all these balls are.
<u>Mark</u>: These are...on, I know (indicating atoms in the diagram) - these are the hydrogen balls and this is the oxygen.
...
<u>Interviewer</u>: That's good. So, the little ones are the hydrogens and the big one is the oxygen?
<u>Mark</u>: Yeah.
<u>Interviewer</u>: Are the hydrogen atoms and oxygen atoms stuck together, are they touching each other, or are they loose?
<u>Mark</u>: They are stuck on each other.

Mark has abandoned his belief that water is composed of a mole of oxygen and hydrogen atoms joined by carbon bonds.

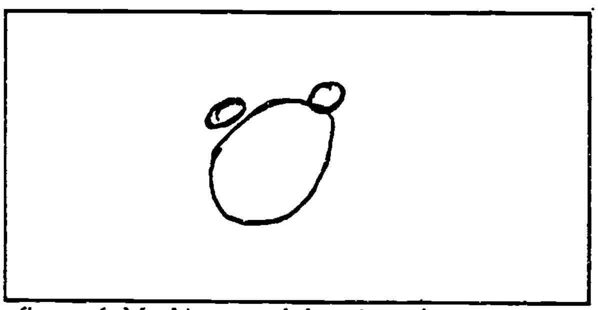

figure 6: Mark's second drawing of a water molecule

As for Mary, the next time she was asked to draw a water molecule, after having seen the simulation only briefly, she was able to draw an oxygen atom with two hydrogen atoms attached to it. She still had misconceptions about water molecules. As she drew the water molecule she said, "The hydrogens can be anywhere on the oxygen atom." indicating that she did not understand that the bond angle was fixed.

Structure of molecular water (ice/liquid/vapor):

After working with the software for two weeks, Mary was able to draw and explain how the water molecules were arranged in the ice and liquid states. Figure 7 is a drawing Mary did of molecular water one week after she had used the simulations for one two hour session. The following dialog is from a post interview with Mary after four two hours sessions working with the simulations. Notice that she has abandoned her idea that water in the gas phase is composed of free hydrogen and free oxygen.

> _Mary:_ *When I was trying to guess how it would turn to a gas and I was wondering if they split apart and that didn't happen. They stayed the same way. they're supposed to be but they are just like loose. So that was the gas.*
> _Interviewer:_ *So when you say you thought they would split apart what do you mean?*
> _Mary:_ *When the hydrogens and the ...oxygens , when they split apart. I thought that the molecule itself would split apart but ...it wasn't that. Now that I think about it I think that's kind of a stupid answer.*

Mary has abandoned her belief that the oxygen and hydrogen molecules will separate in the gas phase. She has also come to a better understanding of how the molecules are bonded together via the hydrogen atoms as the following transcript suggests.

> _Interviewer:_ *Go ahead and look at the ball picture.*
> *Diane follows her instructions and switches to the ball representation. Mary and Diane look at the screen.*
> _Interviewer:_ *Have a look at this. This is ice. How is it different from what you were looking at a few minutes ago?*
> _Mary:_ *This is ... Molecules are joined together by the hydrogen atoms. Other ones were separated.*
> _Interviewer:_ *You can rotate the box and see whether oxygen stuck together too.*
> *Diane switches to the stick picture, rotates the box and switches back to the ball representation. They look at the screen.*
> _Interviewer:_ *Are oxygen stuck together or just little hydrogen?*
> _Mary:_ *No. They stuck from hydrogen.*

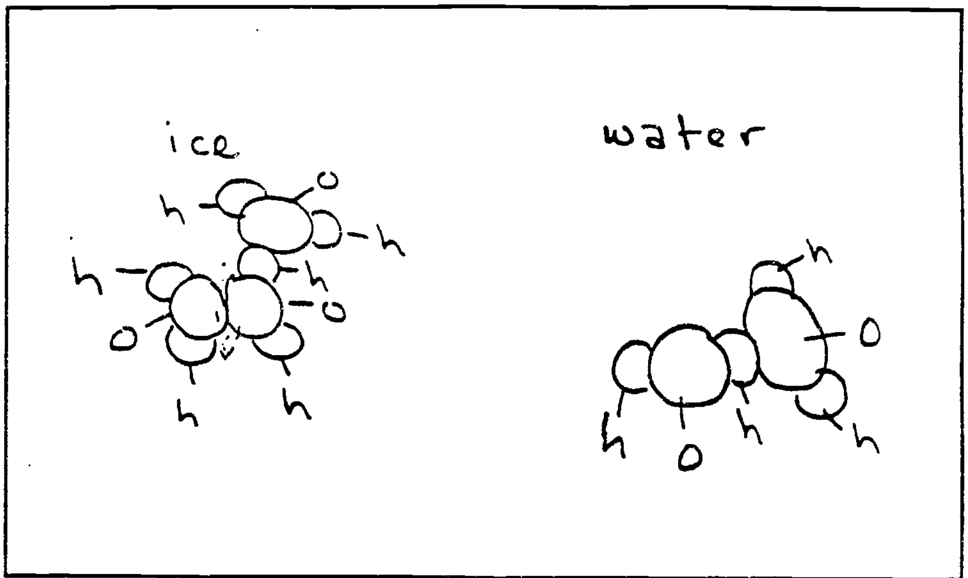

figure 7: Mary's sketches of the molecular structure of water in the solid (ice) and liquid states one week after exploring the RISC-based simulations.

Figure 8 shows Mark's second drawing of molecular water in all three states done one week after using the simulations for one two hour session. While he still believes that ice is more dense than liquid water, his conceptions regarding the hydrogen bond network are markedly improved. Here is a portion of field notes taken from the videotape of his interview.

> *The interviewer asks Mark where the molecules are stuck together in ice. Mark points to places where a hydrogen of one molecule is touching the oxygen of another molecule. He says he does not think that the oxygen would be stuck together. The interviewer asks how liquid is different from solid. Mark says that the solid is clumped and the molecules in the liquid are not as close together. He says he is not sure what happens in the gas but he thinks the molecules should be more spread out.*
>
> *Interviewer: Are the molecules any bigger?*
>
> *Mark: I don't think they're any bigger, just more spread out.*
>
> ...
>
> *Interviewer: In the gas phase are they still stuck together, the way they are in the liquid and ice?*
>
> *Mark: Looser bond. Some are stuck and some are not.*

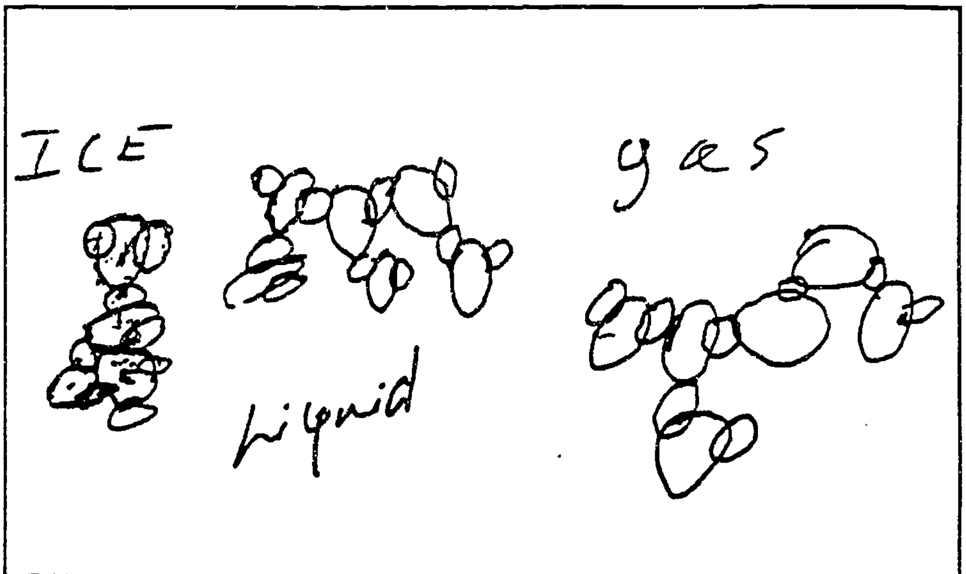

figure 8: Mark's sketches of molecular water in the solid (ice) liquid and gas (steam) states one week after using the RISC-based simulations.

Kevin's understanding of the molecular structure of water has also improved, as demonstrated in figure 9. He draws the oxygen and hydrogen atoms in each water molecule and he draws an open structure for the solid phase. His diagram, however, does not show the hydrogen bonds accurately. Each oxygen atom should have two hydrogen atoms bonded to it. A hydrogen bond forms between water molecules when one of those hydrogen is bonded to the oxygen atom of a different water molecule because of the electrical polarity of a water molecule. Kevin's diagram does not show enough hydrogen atoms for the number of oxygen atoms he has drawn.

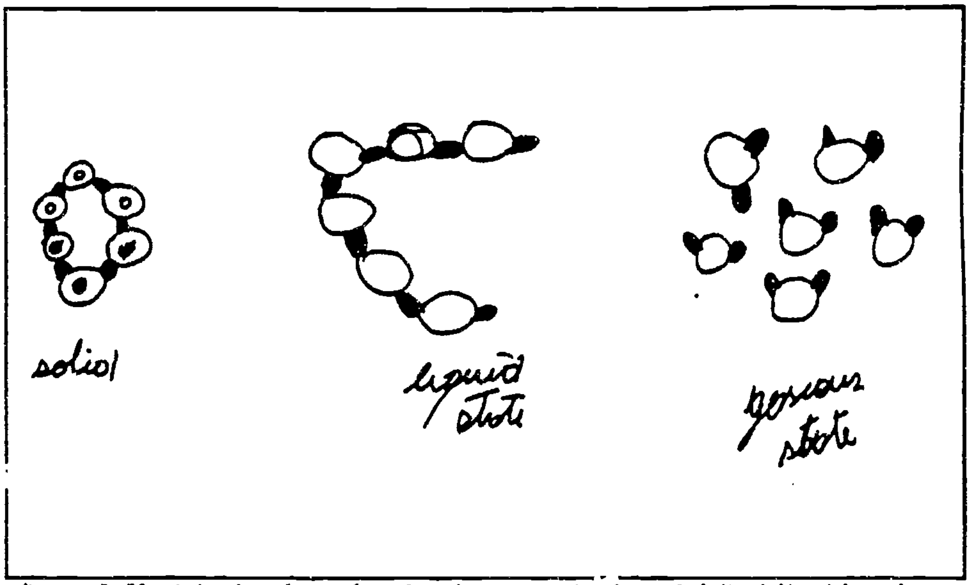

figure 9: Kevin's sketches of molecular water in the solid (ice) liquid and gas (steam) states one week after using the RISC-based simulations.

Temperature and kinetic energy:

The water simulation also addresses the relationship between the kinetic energy of particles and their temperature. Although Mary had not yet learned about kinetic energy in school, she was able to qualitatively describe the relationship between speed and temperature. The following is a portion of the demonstration interview with Mary.

> *<u>Interviewer:</u> Mary, what are you changing?*
> *<u>Mary:</u> Temperature.*
> *<u>Interviewer:</u> What happens?*
> *<u>Mary:</u> They move faster. (Mary changes the temperature one more time. She then decreases the temperature. She looks at the screen attentively.)*
> *<u>Mary:</u> They move more slowly.*

Mary has discovered the relationship between the speed of the water molecules and the temperature of the system. This relationship is not something that was told to her by the interviewers but something she discovered for herself.

<u>What helped</u>

Visualization:

Visualization is a powerful tool to help students who have difficulty in science as well as those who are successful in traditional classrooms. Visualization helps students develop mental models and gives them a conceptual framework to which they can attach the abstract ideas they have already learned or are about to learn in school or from textbooks.

During the course of our demonstration interviews we asked the students how they like using the computer simulations and how this compared to their science classes at school. The answers they gave were very revealing and indicated that they appreciated the power of visualization. Kevin and Mark said the following.

> *Kevin: A picture is worth 1000 words.*
> *Mark: If a picture is worth 1000 words, this program is worth 1,000,000 words because I can control this picture.*

Mary expressed herself in the following way.

> *Mary: When you are in school and they're just up there teaching you stuff but you really don't know what they're talking about... Let's say two views, one is actually knowing it yourself and one is having somebody tell you. So if you could really look at the stuff yourself you could understand it better than just the teacher up there. He says it's like that and you say, 'okay it's like that,' but you really don't believe it until you really see it yourself.*

A male honors student from a suburban school said something very similar. He told us he liked these simulations better than a book because he could visualize the molecules and perform experiments.

The visualization aspect of the simulation allows students without strong backgrounds in math to feel some success in science. There is no knowledge of math required in order to learn the concepts addressed in the simulation. Diane and Mary, the ninth grade students had especially poor math backgrounds yet they were successfully able to learn about the structure of water and even about the potential energy of water molecules with respect to ions in solution. This is true conceptual science.

Multiple representations:

Scientist build and use models every day. More than one model or representation can exist for the same concept. Scientist use multiple representations or models to help them understand various aspect of an idea. It is the multiple representations (ball and stick) of the water molecules in the computer simulations which help the students come to a more complete understanding of the molecular nature of water. The ball model helps the students to understand the three dimensional nature of the molecule. The stick model helps them to see more clearly the flickering hydrogen bonds. They are both useful in their own way.

In the demonstration interviews we found that all of the students continually switched back and forth between the two representations. Unfortunately at the time the interviews were done the ball model was static only. The stick model was dynamic. Nevertheless the students would continually update the ball model as the stick model changed. When Mark and Kevin were investigating the water simulation Mark would change a parameter such as density and then update the ball model to see what the "real thing" might look like. He told the interviewers that he felt it was easier to tell what phase the water was in from the ball model.

Mary used the multiple representations to prove that there are no bonds between adjacent oxygen atoms and that water molecules form a network from the hydrogen of one molecule to the oxygen of another. She would look for a place in the ball model where two oxygen molecules looked like they might be touching. She would then find the same spot in the stick model and look to see if there was a blue line indicating a bond between those same two atoms. By doing this for quite a while she determined that indeed the bonds only existed from hydrogen to oxygen.

Interactive control of parameters:

Being able to test ideas is an important part of learning. Students need to prove for themselves that an idea they have is or is not plausible. It is usually not enough for the teacher to simply tell them. Without simulations, however, it would be impossible to show a student that, for example, raising the temperature of a container of water molecules would cause them to move faster. With a computer simulation the students have the control they need to change their misconceptions.

By controlling the parameters available to them, Mark and Kevin are able to explore the consequences of changing the temperature and pressure. They are able to discover for themselves what happens to the water. The following is part of a demonstration interview with Mark and Kevin. Peter is a graduate student.

> *Peter:* *Yeah, you should try that, don't believe me! Grab hold of the temperature and change it. Put it all the way up.*

Mark: (changes the temperature from bottom to the top) It's all the way up. (pause) The box expanded.
Peter: Did you notice the difference?
(long pause)
Interviewer: What do you see happening?
Mark: They are going...away from each other.
Interviewer: Is it behaving the same way it did before, or does it seem different now?
Mark: It is different.
Interviewer: How?
Mark: Now the...each one of these...among these sticks, they are all...they move quicker now. And they are all going in different ways and they are closer. (puts the temperature down)
Interviewer: So what do you think is going to happen to them?
Mark: It should move back, it should move closer. These just got...touched each other - now they go away again. Do you know how quickly the ...
Interviewer: What was your question?
Mark: I was just wondering how quickly would the things change. (pause) There are slower movements now.
Interviewer: So what happened when you lowered the temperature all the way down?
Mark: It slowed down.

The interactive nature of the simulation allows students to answer questions they generate themselves. In the following section of a demonstration interview, Kevin wonders whether the simulation will show a gas.

Kevin: Can you show us the molecules in the gaseous state?
Peter: Yeah.
Kevin: Have we seen it yet?
Peter: Can you think of how you'd make the gas state?
Kevin: Boil the liquid.
Mark: Yeah.
Kevin: Boil the water.
Peter And how do you do that?
Kevin: Increase the temperature.
Peter: Temperature up. (Mark switches to stick mode and increases the temperature.) Here you go.

Interviewer: And how would you guys know if it is a gas? What is the way to tell?
Mark: By the...movements, a lot of movements. It is like the ...it is like before when it was at high temperature. There were again a lot of movements - as I drop the temperature, it just slows down... Something will happen.

Later on Kevin says the following about why he like the simulations.

Kevin: You can actually see it and experiment with it. At school they might just tell you but you don't get to try your own thing like different temperature, different pressure and all that stuff.
Interviewer: Why doesn't just showing you a picture at school help?
Kevin: You don't get to try out all the possibilities there are.

Mary had a misconception that the water molecules would break apart into free hydrogen and oxygen in the gas phase. She raised the temperature in an attempt to break apart the molecule. When that did not work she varied the pressure. Finally she convinced herself that, in fact, the water molecules remained intact in the gas state. It was through her control of the parameter that she was able to make that discovery.

Debate with partner:

Having a partner to work with seemed to help the students refine their conceptions. Through discussion with a partner students are forced to articulate their beliefs. They can them compare the merits of their view with those of their partner. A discussion then develops which can become fairly lively if the students have different ideas and are each convinced that they are right. Eventually each student must make a decision based on the discussion and the evidence from the computer simulation as to whose view is correct.

A good example of this is Mark and Kevin. They had both independently drawn pictures of solid, liquid, and gaseous water for the researchers. A week after their second drawings (figures 8 and 9) they were given their drawings and asked to discuss them. The following is taken from field notes of the videotape.

Kevin thinks that Mark's drawing is wrong because he sees three hydrogens for every oxygen. Mark argues with him saying that he is looking at the drawing incorrectly;y and there are only two hydrogens for each oxygen. Mark draws circles *around his individual water molecules to prove his point. Kevin counts the number of oxygens touching each oxygen to prove his point. Mark then uses the simulation to show that the water molecules are connected by hydrogen atoms and therefore it looks like there are three hydrogens attached to each oxygen. Kevin is convinced when he sees it in the simulation.*

It was through debate with his partner Mark that Kevin came to understand how water molecules are connected.

CONCLUSIONS

Our ongoing research has uncovered serious preconceptions related to the microscopic and macroscopic properties of water. We have documented how the computer simulations help students change their conceptions. From the students themselves we have learned that the simulations work because they are visual and highly interactive. The findings of this study support previous research results which show that computer simulations designed with student preconceptions in mind can help promote conceptual change in students.

The preconceptions we found were similar to those uncovered by Novick and Nussbaum (1981) which were related to how students understand the particulate nature of matter and its relationship to macroscopic properties. We also found preconceptions similar to those found by Griffiths and Preston (1992). They also found no significant differences between the preconceptions held by students with strong science backgrounds and their fellow students who had received little formal science instruction. We found that the WAMNet simulations worked equally well for students with strong science backgrounds as well as students with poor science backgrounds. We have seen students with very poor backgrounds in science come to an understanding of the molecular nature of water and students with reasonably good science backgrounds learn even more. Griffiths and Preston (1992) argue that it is the complexity of the particle nature of matter which makes it difficult for students to conceptualize. Because they have difficulty visualizing it they develop alternative conceptions. With simulations such as these they can now visualize the particle nature of matter and develop more scientific conceptions.

Allowing students control of such visual, dynamic, and interactive simulations empowers them and gives them control of their own learning. It is a true constructivist tool because it allows students to explore their own questions and construct their own meaning. Because of the limitations of the laboratory in which all traditional experiments must be done, students were never able to "see" the world on the molecular level. These simulations allow the students not only to see static pictures of the molecular level but to actually experiment with dynamic, three dimensional, models. They can raise the temperature and actually see the molecules move faster, not just listen to their teacher tell them that the molecules move faster. They can watch a salt dissolve and see how the water molecules react to the presence of the ions. It is a "conceptually enhanced" computer simulation, to use the terminology of Snir, Smith, and Grosslight (1988).

We have seen that students who use the simulations change their conceptions about the molecular nature of water. One might ask, so what? Now students can draw an accurate picture of a water molecule and the structure of water in solid, liquid, and gaseous states but is that really important. The students are demonstrating that they have some understanding of the particulate nature of matter. This is a rather important concept in chemistry. We have shown that computer simulations can help shed light on an area that is difficult to teach because of the lack of good visualization opportunities in the traditional curriculum. Although it is true that right now RISC machines are too expensive for most public and private schools, their cost is falling. Within ten years most schools should be able to afford these machines and then this kind of simulation will be available to them.

An argument could be made that the research staff paid a great deal of attention to the students who came for the demonstration interviews and that might have had some effect on their conceptual development. The next logical step in the research, therefore, is to see how the simulations work with whole classrooms of students. During the 1992-1993 school year such a classroom has existed at a suburban Boston high school. Although our data from that school is, at this time, still very preliminary the experience of the teacher and the students has been positive.

The preliminary research that we have done shows that placing computer simulations into the classroom necessitates changes in classroom management and teaching style. Further research needs to be done on exactly how the classroom and teacher change. Like any tool, these computer simulations can be use properly or improperly. In order for teachers to use the simulations to their fullest they will need to learn more about constructivist theory. Using the simulations can force a teacher to pay greater attention to the weaker students as the stronger ones will take off on their own. A classroom in which groups of students are working on projects is also a less threatening environment for a weaker student to ask for help. Using simulations should be helpful for both strong and weak students. This is another area for further research.

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