Interactive Educational Multimedia, Number 11 (October 2005), pp. 212-226
http://www.ub.es/multimedia/iem

Improving Physics learning with virtual environments: an example on the phases of water

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Abstract

Usually students have misconceptions on the microscopic structure and behaviour of matter. In order to overcome these difficulties computer-based worlds seem useful to visualize physical and chemical processes allowing for a better conceptual understanding. Since more 3-D virtual environments need to be explored and evaluated in science education, we have built a 3-D virtual environment – "Virtual Water" – to support the learning of Physics and Chemistry at the final high school and first-year university levels. It is centered in the microscopic structure of water and explores concepts related to water phases and the transitions between them.

Keywords

Phase transitions, misconceptions, computer, pedagogical visualization, virtual reality.

Introduction

In Physics and Chemistry one has to consider the macroscopic and microscopic worlds and to be able to alternate between them (sometimes we have to take both simultaneously). This is not easily achieved by high-school or even university students, who have unclear or even misconceptions on the microscopic structure and behaviour of matter in its different states of aggregation. A possible explanation of this problem lies in the fact that most experimental information comes from macroscopic observations while explanatory theories are based on atoms and molecules, the elements of an invisible world which has, in large measure, to be imagined.

Several works (see Table 1 for a synthesis of the misconceptions found by several authors), addressing different learning levels, have been made to identify and understand students' misconceptions in Thermodynamics and Statistical Mechanics with respect to phases and phase transitions. We highlight the following:

- **Griffiths and Preston (Griffiths & Preston, 1992) showed that Canadian students at advanced high school level students tend to transfer to the microscopic world some properties observed in the macroscopic world.**
- Ryan (Ryan, 1990), in a study with first-year college American Physics and Chemistry students, analyzed whether students were able to characterize and distinguish the different phases of matter. He concluded that students tended to classify phases according to the sizes of the constituent particles (as water changes phase, from gas to liquid and them to solid, its particles decrease in size).
- Benson, Wittrock, and Baur (Benson *et al.*, 1993), studying a large group of American Physics, Chemistry and Biology freshmen, found that students understand gas as a continuum behaving very much like a liquid.

Table 1. Some misconceptions concerning phases and phase transitions.

Phases

Gas	Spacing between particles is small in the gaseous phase (Benson *et al.*, 1993; Krnel *et al.*, 1998; Bar & Galili, 1994).
Liquid	Liquids are wet substances which can flow (Lee *et al.*, 1993).
Solid	Molecules are very close to each other so that no empty space exists between them. Molecular binding is due to some external agent (Griffiths & Preston, 1992).

Phase transitions

Solid-liquid	When ice is heated up, heat expands each molecule, leading to its separation (Griffiths & Preston, 1992). In the liquid-solid transition the weight of the sample increases while in the inverse process the weight decreases. Hydrogen and oxygen combine to form water (Bar & Travis, 1991).
Liquid-gas	When water boils the bubbles that appear are made of oxygen or hydrogen (Bar & Travis, 1991).

Molecular dynamics

Temperature	Molecules are hot or cold according to the phases they belong to (Griffiths & Preston, 1992).
Molecular behavior	Students find difficult to foresee the molecular behavior in different phases (Williamson & Abraham, 1995) and to distinguish different phases (Ryan, 1990).

Molecules

Shapes	Particles have different forms in different states: gas molecules are round, liquid molecules have irregular forms, and solid molecules are cubic (Haidar & Abraham, 1991; Griffiths & Preston, 1992; Krnel *et al.*, 1998).
Speed	The speed of a molecule is determined by its size. If a molecule has more space to move around its speed will be larger (Griffiths & Preston, 1992).
Size	The diameter of the molecules decreases progressively in the successive transitions from first solid to liquid and then to gas (Griffiths & Preston, 1992).
Weight	The weight of a substance changes in phase transitions (Krnel *et al.*, 1998).

The structure of matter is an adequate topic for pedagogical visualization and one is tempted to think that computer simulations may help to deal with at least some of these cases. Animated pictures may help to visualize the microscopic motions that occur in the gaseous and liquid phases of water. In fact, various authors (Trick & Pylyshyn, 1994; Stoney & Oliver, 1999) have defended the regular use of computer simulation and visualization in Physics and Chemistry teaching. They further argue that students should be given an active role in using these tools (Smith, 2001).

However, the use of computational means in Physics Education has been standing mainly on 2-D representations. Only recent advances in visualization and computer technologies have created new possibilities: the visualization of 3-D objects and data became increasingly important in learning many subjects. For example, the Water program, developed by the Virtual Molecular Dynamics Laboratory of the Boston University (http://polymer.bu.edu/vmdl) simulates the behavior of water molecules in 3-D. This application introduces final high school and college students to the microscopic dynamics of water by showing them how various water properties arise from hydrogen bonds.

It is probable that the change from 2-D to 3-D helps to increase the understanding of processes which, in reality, take place in full space. The possibility of interactivity is also likely to help. One of the most promising means to support advanced learning environments for science education is virtual reality (Kim *et al.*, 2001). This is a computer interface characterized by a high degree of immersion and interaction, which may make the user believe that it is actually *inside* the artificial environment. In a perfect virtual environment, a user would be completely unable to determine whether it is experiencing a computer simulation or the real world.

Although the concept of virtual reality has been used for more than thirty years, only recent progresses in hardware and software brought this technology to within the reach of ordinary users. An advantage of virtual reality in science education is its ability to visualize microscopic processes and to immerse learners in them. For example: a picture or a movie may show students the internal structure of ice, but only virtual reality allows them to "enter" inside and observe it from any viewpoint; or an animation can illustrate the solid-liquid phase transition, but virtual reality provides students with a much stronger sense of "being there". This realism has a great potential to increase the effectiveness of educational simulations.

Our purpose

We have developed "Virtual Water", a stereoscopic virtual environment to support the learning of some concepts of Physics and Chemistry by students who are at the final year of high school or at first-year of university studying the effect of 3-D interactive simulations on students' visualization of phases and phase transitions of water. Our virtual environment is centered in the microscopic structure of water and, among others subjects (such as atomic and molecular orbitals), allows to explore phases of matter and phase transitions (http://aguavirtual.mediaprimer.pt).

We have shown (Trindade et al., 2002) that "Virtual Water" helps students with high spatial aptitude to acquire better conceptual understandings of some thermodynamical concepts (solid, liquid and gaseous phases, and transitions between them). Only some parameters of the virtual environment (interactivity, navigation and 3-D perception) have shown to be relevant and only for some of the referred topics. Although some results have been described elsewere (Trindade et al., 2002), we intend with this paper to discuss some of the students' answers before and after using our virtual environment, in order to stress the pedagogical utility of our software to overcame conceptual difficulties with phases and phase transitions. This study is essentially qualitative.

Let us briefly describe the development of our software. For model design we used the free software PC Gamess (http://www.msg.ameslab.gov/GAMESS/ GAMESS.html), which performed the calculations on the water molecule, and Molden (http://www.cmbi.kun.nl/~schaft/molden/ molden.html), for the molecular representations. For model development and optimisation we used commercial software packages (Mathcad and 3-D Studio Max) and for implementing the molecular dynamics algorithm Visual C^{++}. Concerning the definition and creation of the virtual scenarios WorldToolkit (from Sense8) was employed. Finally, for visualizing the stereo virtual environment we used appropriate glasses (with stereo capabilities) and graphics board with stereo output.

The minimal hardware requirements for "Virtual Water" are a Pentium III processor, 128 MB of RAM, 150 MB of free hard disc, graphics board accelerator, and Microsoft Windows NT 4.0 or higher. Upon request we may distribute our software for educational purposes.

Methodology

According to Erickson (Erickson, 1985), observations of student's attitudes and interviews are adequate methods to perform descriptive studies like the present one. To detect differences between conceptual comprehension without and with software visualization oral answers given by students were analysed (we video taped oral interviews). The idea was to compare the students' answers before and after software view to find a correlation between conceptual comprehension and computer use. Our dependent variable is the level of conceptual comprehension on phases and phase transitions of water, while our independent variable is the use of 3-D interactive computer simulations.

Our qualitative study involved 20 first year students attending Physics, Chemistry, Industrial Chemistry, Physics Engineering and Civil Engineering courses at the University of Coimbra, Portugal. The sample is the same in a previous report (Trindade et al., 2002). Phases and phase transitions had been taught at an introductory level in their courses since these subjects belong to the "General Chemistry" syllabus (Chang, 1998).

Results

The chosen set of scenarios focused on the molecular dynamics of water in the gas, liquid and solid phases. In all of them, 72 molecules were seen in a 3-D box; phase transitions occurred when the student changed the temperature or the pressure. We hoped that our computer scenarios provide a deeper understanding of phases and phase transitions at the microscopic level. Students were asked to answer some questions on that topic, before and after seeing "Virtual Water".

It is clear from the observation of our virtual environment that, in any phase, empty intermolecular space is present. This space is smaller in the liquid phase than in the gas phase. It is therefore apparent that the water density is different in these two phases.

Gaseous phase

In this scenery we see 3-D animations of molecular dynamics, which correspond to a temperature slightly above 100 ºC and to atmospheric pressure (Figure 1). The most relevant features of the water molecules are their high mobility and their difficulty to form intermolecular bonds.

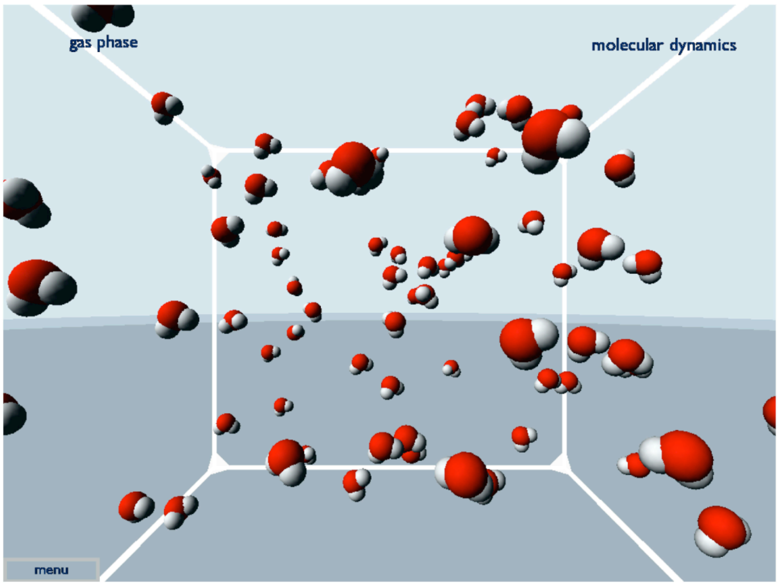

Figure 1. **Gaseous phase at atmospheric pressure. Molecules have very high mobility. The dark spheres represent oxygen atoms while the gray ones represent hydrogen atoms.**

A question on the gas phase we have raised and some representative answers given by students before and after software use are the following.

Question 1: Why is the volume occupied by the molecules so large?

Typical answers:

a) Before software use: “*It is like having a gas in a balloon. The molecules have a lot of energy and move without any restrictions*”.
After software use: “*When the temperature increases the molecules tend to spread*“.

b) Before software use: “*Because nothing hinders the motion of molecules. Since there are no forces, particles move with maximal energy*”.
After software use: “*Because the temperature is larger in the gas phase being the pressure constant. The molecules received a lot of energy*”.

In both answers before software use, students recognize that, in the gas phase, particles have high energy and mobility. These answers, like others, although essentially right, are somewhat vague. After computer visualization students’ ideas are related to the temperature increase (at constant pressure).

Gas-liquid transition

By decreasing the temperature at constant pressure, the molecules form intermolecular bonds and loose their mobility (Figure 2). The increase of density and the emergence of some molecular clusters are clearly noticed.

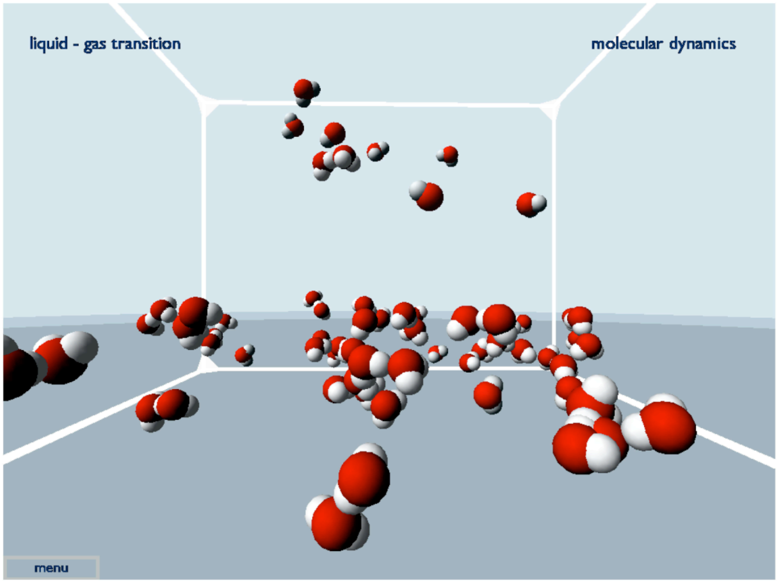

Figure 2. Gas–liquid transition: the most relevant phenomena are decrease of molecular mobility, formation of intermolecular bonds and increase of density.

A question and some student's answers on the gas-liquid transition are the following.

Question 2: Is there any change of the molecules?

Typical answers:

a) Before software use: "*They become larger*".
After software use: "*The molecules do not change but their speed changes*".

b) Before software use: "*The molecules are the same, but now, with the increase of pressure, they tend to increase their size*".
After software use: "*They look the same but now are closer*".

Answers a) and b) before software use are wrong. Students confuse molecular mobility and molecular size (a typical misconception is that

small objects have higher mobility). However, after software use, students understand that the size of molecules is unchanged in the phase transition.

Liquid phase

If we continue to lower the temperature but keep the pressure constant we obtain the liquid phase (Figure 3). The phenomena which have been observed in the latter phase transition become more intense, leading to more intermolecular bonds, less molecular mobility and larger density.

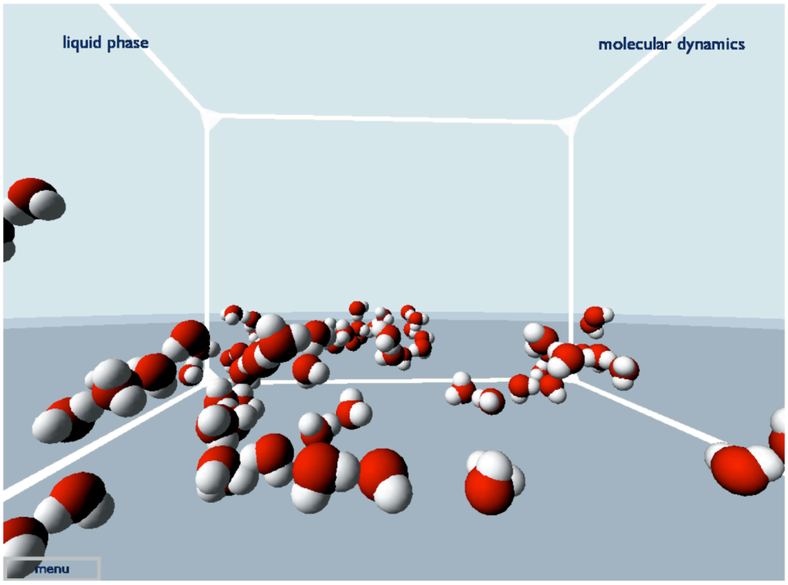

Figure 3. Liquid phase: Intermolecular bonds are formed, molecular mobility is reduced and density increases.

Again, we have asked students about this phase before and after careful computer visualization.

Question 3: Is there any change of the weight of the molecules?

Typical answers:

a) Before software use: "*Yes. They lose speed and also become larger so that they take more space*".
After software use: "*The individual molecules (H_2O) have the same atoms. The weight will be the same. However the $2H_2O$ molecule is heavier than H_2O*".

b) Before software use: "*The weight should increase because they are losing speed and are falling*".
After software use: "*The molecular motion is now slower. But the water molecules remain the same. I think that their weight is the same*".

These answers before software use show that students do not understand the conservation of mass (and, therefore, weight) in the process of condensation. However, the idea of mass conservation becomes clear after computer visualization.

Liquid-solid transition

If the temperature further decreases, the mobility of the molecules becomes even smaller and small pieces of ice structures show up (Figure 4).

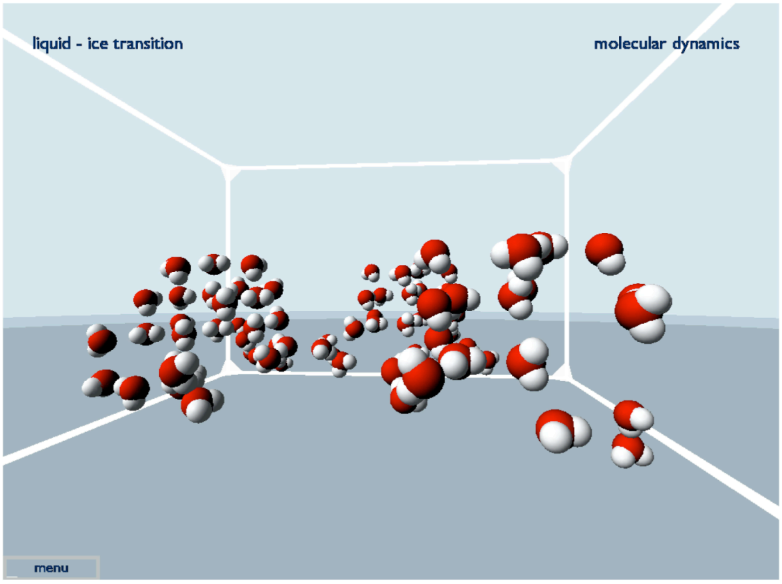

Figure 4. Liquid–solid transition: the mobility of molecular aggregates decreases and new intermolecular bonds arise so that the ice structure slowly emerges. Although for our small number of molecules the gravity effect is not perceptible, in the transition from the liquid to the solid phase we placed the molecules in the box's bottom.

A question and some students' answers before and after view of the liquid-solid transition in the computer are the following.

Question 4: Explain what happens to the density in this transition.

Typical answers:

a) Before software use: "*The density increases because the weight increases*".
After software use: "*The density increases because the molecules are closer*".

b) Before software use: “*The molecules join and, since the set is heavier, they fall down. The density has therefore to increase*”.
After software use: “*The density increases. The molecules are now mainly restricted to the bottom of the box*”.

Some students mix together the concepts of weight and density. However, after software use, more students seem to understand the concept of density.

Solid phase

The temperature is reduced to 0 ºC, when the hexagonal structure of normal ice (Ih) (Figure 5) appears in its full extension. Molecular translational and rotational motions are now almost absent.

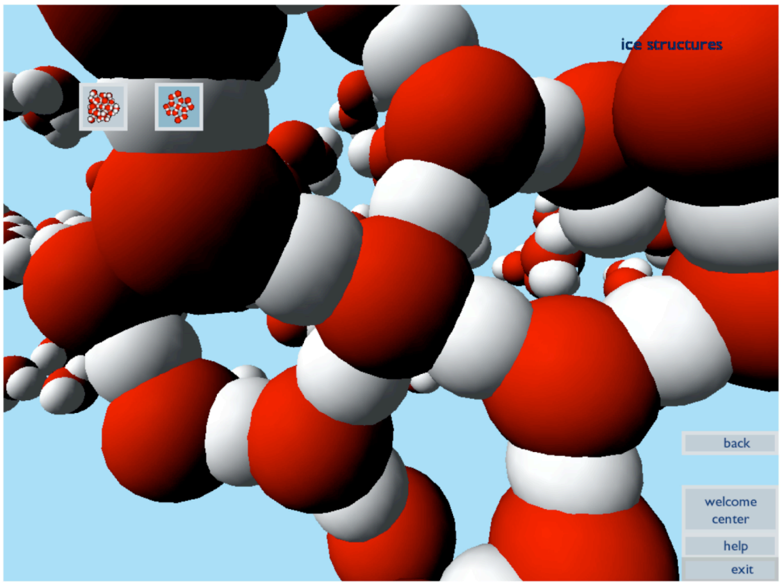

Figure 5. **Structure of normal ice.**

A question and some answers relative to the solid phase are the following.

Question 5: Explain the structure of normal ice based on molecular binding.

Typical answers:

a) Before software use: “*The structure of ice is a ring with five or six molecules of water*”.
After software use: “*The structure is a hexagon. Oxygen is bonded by four hydrogen atoms*”.

b) Before software use: “*Molecules are all compressed forming plane surfaces*”.

After software use: "*Hydrogen and oxygen atoms are bond together. There is a lot of space between atoms*".

Before computer visualization students do not have a clear idea of the structure of ice. An advantage of computer visualization is its ability to show 3-D representations like that of ice structure. This helped the students to visualize the structure of normal ice. Answers after software use, although not completely accurate, confirm the utility of the visualization process. In particular, the larger intermolecular spacing in the solid phase was recognized (water is a peculiar liquid with respect to that feature).

All previous students' statements were oral comments. To make the description more precise we have made a simple statistics of the students' conceptions. In order to enable quantitative statements, students' conceptions were classified on an ordinal scale. The array of variable classification ranged from 1 (dead wrong) to 5 (completely right), according to Table 2, as done in previous studies (see *e.g.*, Haidar & Abraham, 1991).

Table 2. **A categorization scheme of student's conceptions.**

Variable classification	Degree of understanding
1	No response ("I do not know" or "I do not understand")
2	Incorrect responses with wrong terms
3	Incorrect responses using a moisture of correct and wrong terms
4	Responses that use the correct terms but do not match scientific conceptions
5	Responses that use the correct terms and match scientific conceptions

Figure 6 shows the traditional boxplots concerning the comprehension of phases and phase transitions without software use and after computer visualization. As we can see, the results are somewhat better with software (there were more correct answers). For the phases concepts the mean score after software use is 4.30, with a 0.66 standard deviation, while for the phase transitions concepts the mean score is 4.20, with a 0.62 standard deviation.

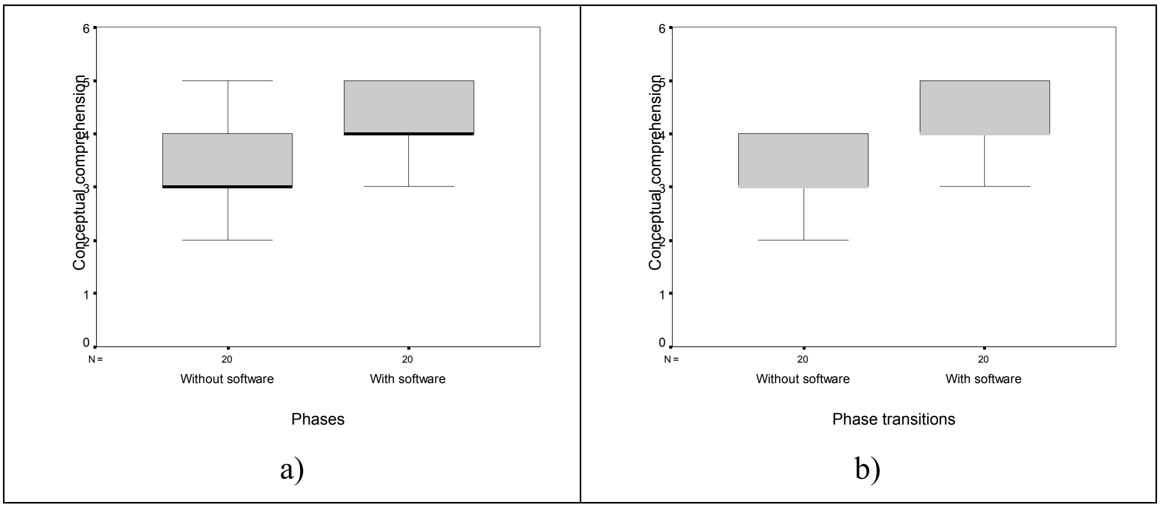

Figure 6. **Boxplots for conceptual comprehension without and with software: a) phases and b) phase transitions.**

Using the Spearman test (at a confidence level of 5%) we found correlations between conceptual comprehension and some characteristics of computer visualization, like interactivity and 3-D perception (Table 3). We found a stronger association for conceptual comprehension of phase transitions.

Table 3. **Correlations between computer visualization and conceptual comprehension.**

	Computer visualization	
Conceptual comprehension	Interactivity	3-D perception
Phases	0.473 ($p<0.05$)	0.552 ($p<0.05$)
Phase transitions	0.769 ($p<0.01$)	0.707 ($p<0.01$)

One of the values of virtual reality is its ability to give substance to abstract concepts. We think that this value was illustrated in our project. We distributed a questionnaire with open questions about the software and the students' answers were, in general, very enthusiastic. Some of the students' comments are the following:

- "*When I work on a Physics or Chemistry problem for an hour, all I have to show for my efforts is a number, which doesn't always mean anything to me. This program gave me a chance to see the behaviour of water molecules for the first time*".
- "*This visualization will stay with me*".

- "*This experience will stay in memory much longer than any notes or lectures*".
- "*Very good form of learning, a good complimentary device*".
- "*The software is especially good for 3-D behaviours*".
- "*It is easier to understand things when you can visualize them*".

Furthermore, students after having explored 3-D molecular motion and its relation to macroscopic properties, appeared to show an increased motivation for studying the theory behind the molecular dynamics they have seen.

Conclusions

We recognized in most of our student's answers, given before software use, errors which have been previously identified by various authors. For example, the answers to question 2, on the shape of molecules, correspond to misconceptions focused by Haidar and Abraham (Haidar & Abraham, 1991), Griffiths and Preston (Griffiths & Preston, 1992), and Krnel, Watson and Glazar (Krnel *et al.*, 1998). And the answers to question 3, on the weight of the molecules in the liquid phase, match misconceptions studied, for instance, by Krnel Watson, and Glazar (Krnel *et al.*, 1998) (see Table 1).

"Virtual Water", our graphical visualization tool with 3-D animations, showed its utility to increase students understanding of phase transitions (gas-liquid and liquid-solid), overcoming their previous misconceptions. The same was achieved, although in a less degree, regarding the gas, liquid and solid phases themselves. The most important characteristics that contributed to students' conceptual comprehension were interactivity and 3-D perception.

Finally, we would like to add that we are aware of the limitations of the present study. Confounding factors may influence the results, *e.g.*, the novelty of the experimenting hardware and software.

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