VISUALIZATION IN CHEMICAL EDUCATION

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ABSTRACT
In this present study, we investigated the capabilities of computer-based construction tool *Construtor* that allowed students to build virtual molecular models and view multiple chemical representations using computational molecular simulations. *Construtor* integrates various supports for learning of molecular structure meaning based on representation levels. The findings also suggest that computer based models can help students to make translations among representation levels.

KEYWORDS
simulation, visualization, molecular objects, software.

INTRODUCTION

As information and communication technologies (ICT) tend to take up more and more aspects of our lives, education is pushed ahead to develop new methodologies to mediate the appropriation of ICT and their correlated ways of acting. The development of software now comes to the help of students, revealing processes and principles that until now could be presented just theoretically. From the point of view of chemical education, it is well documented that students have difficulty to learn the symbolism and to use molecular representations to solve problems.

This paper reports on the development of a tool (*Construtor*) to foster the construction of chemical representations by students at secondary school with the aid of a computer-based visualizing interface, that provide students to build and visualize representations of chemical structures.

VISUALIZATION

Chemistry is a visual science. Visualization plays a major role in chemists' daily practices. To investigate natural phenomena through ideas of molecules, atoms, and subatomic particles, and the relationships amongst them, chemists have developed a variety of representations, such as molecular models, chemical structures, formulas, equations and symbols (Hoffmann and Laszlo, 1991).

Visualizations have also been used for communicating concepts to chemistry students. Secondary school and college chemistry curricula and textbooks use a variety of visual representations to introduce fundamental chemical concepts (Noh and Scharmann, 1997).

Chemical representations are usually gathered into three levels: the macroscopic, microscopic and symbolic levels (Johnstone, 1993; Gabel and Bunce, 1994).

- ✓ Macroscopic – this level refers to picture or diagrams that represent observable phenomena;
- ✓ Microscopic – this level refers to models or other visual displays that depict the arrangement and movement of particles;

- ✓ Symbolic – this level refers to symbols, numbers and signs used to represent atoms, molecules, compounds, and chemical processes, such as chemical symbols, formulas and structures.

All of them in general represent chemical concepts or phenomena at the macroscopic level rather than microscopic or symbolic levels.

Chemistry teachers and educational researchers have recognized the importance of visualization in chemistry learning. A meaningful comprehension of the many representations used nowadays is a difficult task. Many students are not able to provide equivalent representations for a given representation, and they treat chemical equations as mathematical processes, instead of representations of dynamic and interactive processes (Kozma and Russel, 1997), perhaps because of a lack of content knowledge (Keig and Rubba, 1993) or a lack of visual spatial skill (Tuckey, Selvaratnam and Bradley, 1991).

Students are frequently unable to make translations among formula, electron configuration, and ball-and stick models (Furio et al., 2000). They are also unable to explain properties of compounds and chemical phenomena based on the particle matter nature (Garnet et al., 1995). Some authors interpret this learning difficulty as need of the rapid transference among the tree levels of representation (Johnstone, 1991; Gabel et al., 1994). It is more difficult for students to understand the microscopic level and the representation of the symbolic level. Because of this barrier, students' thoughts and explanations tend to rely on sensorial information (Ben-Zvi, Eylon, Silberstein, 1988).

MOLECULAR OBJECTS

Molecular object is a useful definition to understand how chemical knowledge is constructed. The molecular object is an iconographic entity that serves both for indexation and reference objectives and for mimetizing certain molecular properties, having it the possibility of being simulated by means of a system of equations when the object is disseminated by computer (Giordan, 2005). Lazlo (1993) has also defined molecular objects, but in different terms. For him, the molecular object has a realist basis and the molecular formula would represent it. We are not in agreement with the realist emphasis attributed to the molecule and the concept of molecular formula does not either fit well with the many different ways of representing molecules. For educational and epistemological purposes, the focus on the representation of the molecule, which is materialistic as any object, has a profitable foundation to discuss how chemical knowledge is constructed.

Researches have reported the results of learning when concrete molecular objects have been used to visualize the structural and static aspects of the particle model and chemical change (Copolo and Hounshell, 1995). This sort of visualization has been pointed as one of the most used nowadays, because it simplifies, illustrates and allows the exploration of the structure and the associated chemical process. Nevertheless, these objects are rigid and usually available in limited amount, what restricts its use to small molecules (Barnea and Dori, 1999).

The use of information and communication technologies to visualize virtual molecular objects allows multiple coordinated tree-dimensional representations (Kozma et al., 1996), and helps on their manipulation. Many computational tools are available for experts to visualize and manipulate virtual molecular objects. Many of these tools require advanced knowledge in chemistry, such as molecular modeling, and sometimes also in computational science, like programming languages. These features inhibit the use of such tools in classroom. Few of these tools are designed for novices in chemistry, and among those, one rarely presents real properties of compounds and chemical change .

CONSTRUTOR

Our group developed a dual environment tool named *Construtor* to aid novices in chemistry on the creation and manipulation of virtual molecular objects. This tool is designed to be used through hypertext transference protocol (http) to communicate a server computer, which runs simulations using

a molecular modeling package, and a client computer, running an animation interface. Using a proper animation interface, students can build and visualize two-dimensional animations and three-dimensional simulations of molecular objects from condensed structural formula representations. The animations and simulations are visualized on the same screen, so the students might compare their own representations with those scientifically accepted. Simulations are run using the molecular modeling package Tinker (Ponder and Richards, 1987), and visualized with a plug-in (Chime®), both are free of charge for academic use and widely used by researchers.

The graphical animation environment has been written using the Macromedia Flash® application, which is a general edition tool used to build graphic animations from simple geometric images. The resulting client environment reported in this paper enables novices in chemistry to create static two-dimensional animations and dynamic simulations. Figure 1 shows an example of a composition of windows displayed by the application. In the left side of the picture, it is represented the static bi-dimensional set to represent molecular objects. No movement of molecular objects is still offered in this module of the tool. At this stage, we aim to study the actions of the students with this tool and compare them to actions in which they are using paper and pencil to build molecular objects. Through a tutorial, a narrative poses some activities to the students, as building molecular objects with plastic balls and sticks. because students use it in an initial knowledge stage, just after manipulation of concrete molecular objects and drawing molecular representations in paper and also with the aid of computer-based general drawing tools.

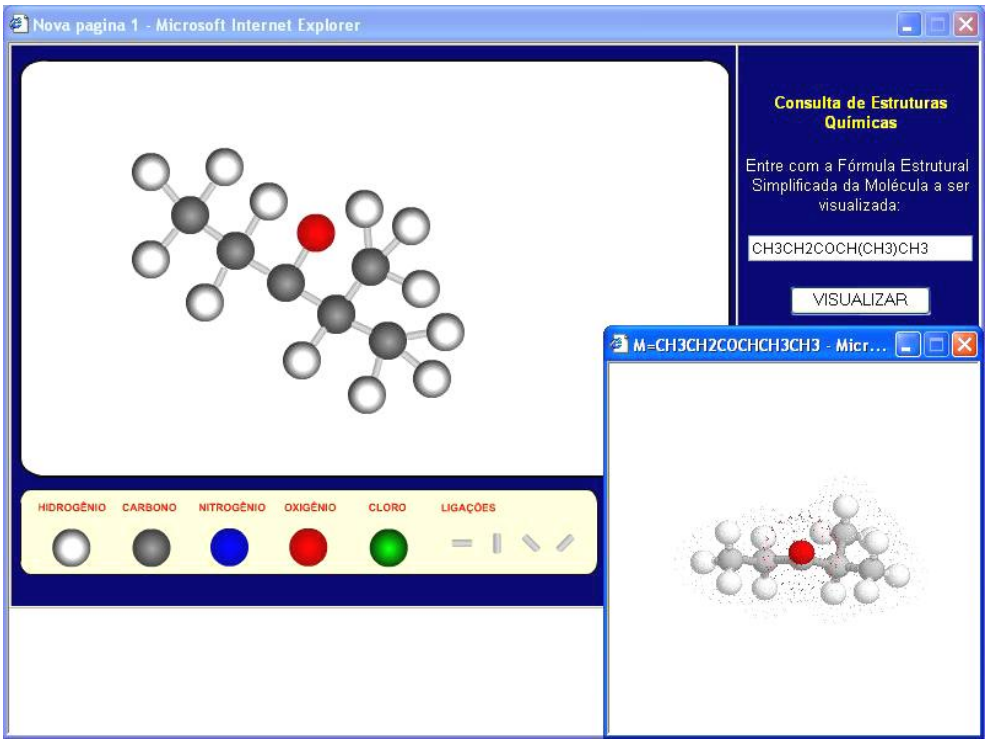

Figure 1. Sample frames from the *Construtor* screen

The simulation environment is shown in the right side of figure 1, and is run both on client and server sides. The client side offers an input field where the user types a sequence of letters and numbers corresponding to a condensed structural formula (i.e. CH3CH2CH3, CH3CH2CH2CHO, CH3COCH2CH3), and also a request-structure button. The server side programs are run on a GNU/Linux environment (RedHat 9.0 distribution). When the user types a coherent formula and clicks on the request-structure button[1], a file containing the corresponding tree-dimensional formula is given back as answer by the server. The is ready to visualize automatically the corresponding tree-

[1] A help interface provides some minimal information on adjustments to regular representation.

dimensional structure whenever it has been previously installed a plug-in (Chime®) in the browser. This input file for the visualization interface is built on the server computer using the molecular modeling package Tinker (Ponder and Richards, 1987).

When the string formula is received on the server side, a script written in Perl language processes and sends it to a program written in ANSI C language, named MODCONSTR. This program interprets the condensed-formula-like string and builds its corresponding three-dimensional coordinates atom file in PDB format , along with a connectivity matrix. This file is automatically submitted by the Perl script to the Tinker Package to optimize the molecular geometry. A second tree-dimensional coordinate's atom file is generated as result, and the Perl script sends it back to the client where it is read by the browser which shows up the simulated molecular object in screen. The first file is written on a linear coordinate's fashion, and doesn't correspond to real structures. It is necessary to optimize the geometry of the corresponding molecular structure using a proper molecular force field. The system does not use any kind of molecular data bank, so the amount of possible structures that can be constructed is proportional to the possible combinations of organic groups up to 100 atoms. *Construtor* recognizes hydrocarbonets, alcohols, aldehyds, ketones and ethers so far, including their unsaturated, branched and cyclic formulas. The time needed to construct an optimized file of about 20 atoms is about one second in a pc-like server of 333 MHz, and will naturally depend on the bandwidth in use.

ACTIVITIES

Computer has the capacity to support molecular-level animations and simulations of chemical phenomena that are not directly perceivable by other means (Giordan, 2005). Integrating this technology not only allows modeling of students thinking at the molecular level, but also permits simultaneous representation of molecular and macroscopic views of phenomena (Russel et al, 1997).

A pilot study has been conducted at Laboratory of Research in Chemical Education - Faculty of Education – University of Sao Paulo (LAPEQ-FE-USP) with students from third year of High school. In this study, we aimed to observe how the students use the interface so we could gather some information on the usability of the interface. For data collection, we have used multiple sources of data including curriculum materials, classroom video recordings, field notes, video recordings of students using the *Construtor*.

According to figure 2 students always work in pairs with the computer because on this way they might talk easily. The interface has been designed to permit students to manipulate plastic molecular objects, while talking to each other about the correct atomic arrangement. In this sense, we could not observe any limitation of the interface, since, as is indicated in figure 2, the students could stop acting with the interface toward building the plastic molecular objects. An important action is the comparision between the plastic model and the computer drawn representation. At this stage, we suppose the students are using the interface to interpret, ie. to compare, their representation in terms of an analogy, that has been introduced by the teacher. This moment of dialogue is extremely important for them to create, elaborate and re-elaborate their concepts of molecule, atoms etc..

Figure 2. Students working in pairs

With the *Construtor* students might create molecular representations, view them from all possible angles and manipulate them more easily than physical ball-and-stick models. The function *visualize* provides students with representations such as ball-and-stick, wire-frame, and space-filling simultaneously. *Construtor* integrates various supports for organic chemistry learning.

Students experienced the *Construtor* in an instructional sequence that integrates molecular representations and problem solving, when learning the concepts of organic chemistry. This kind of activity where student can manipulate models seems important because it can help students to solve problems and to represent chemical concepts at the macroscopic, microscopic and symbolic levels. The findings suggest that the construction of molecular objects with this computerized tool might improve the student's understanding of chemical representations.

In this sense, *Construtor* is a computer-based construction tool that allows the development of activities where students might create and manipulate 2D and 3D molecular representation and also purpose molecular models to account for microscopic and macroscopic levels. Finally, students might improve their ability to translate these representations among them.

When students are able to view and manipulate concrete and computer-based models of molecules, atoms and chemical bonds, these objects help them to construct a more concrete understanding between organic concepts and representations. In the student's opinion, their understanding of abstract concepts has enhanced:

- Before it (the class) I thought different... molecules, are something that I can not see, so it was strange…without meaning, we do not know what is it…
- Now we work on the concrete way, we can see it, we can manipulate it, it seems more concrete.
- We believe in it, we can see an object, adn say: Ah!!! It is built like this, by this way, by this kind of bond…
- It is something new. Form this moment we can see Chemistry on a new way, something more concrete, instead just abstraction or just imagination. It will be very helpful for my school life.

When they view and manipulate these objects they understand the underlying concepts of chemical representation instead while they just watch the demonstrations of those objects by the teacher.

PERSPECTIVES

The next step of the development of *Construtor* is the addition of an interface to generate films made with frames of dynamics simulations. This new functionality of the software will enlarge the possibilities to represent molecular phenomena and especially those correlated to chemical equilibrium. We intend to further develop *Construtor* to integrate different Medias, which might support the students to construct theoretical knowledge and to appropriate a more diversity of chemical representations.

The involvement of the students was very intense during the classes and their results were clearly improved. At any stage of the software design, the users' interfaces are projected to give to students the control over some variables of the system, what is a characteristic of an authentic simulation. Students seem more engaged on this kind activities instead on the class without computer.

Two initial conclusions can be set. First, the use of concrete and virtual molecular objects as learning tools might help students to construct chemical knowledge, and second, computer-based molecular objects support students in translating among different types of representations of chemistry.

The software worked properly, even with many users (18 pairs of students) using it at the same time. The molecular modelling package used to optimize the geometry of the molecular structures didn't require much processing time on a Celeron 333 Mhz, as the time for answers from the server were observed as 1 or 2 seconds.

This study is in an initial stage, as the software is in constant upgrade to perform more kinds of organic structure building. Inorganic structures will be also incorporated in the program algorithm. At this point of the study there is enough evidence that high school students can also use highly capable molecular mechanics programs, used only in scientific applications, with appropriated modifications. We intend to develop the program to perform molecular dynamics under request of students, and give them appropriated variables to modify.

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