CONSTRUCTOR OF MOLECULAR OBJECTS: AN INTERFACE FOR CREATION AND VISUALIZATION IN COMPUTING ENVIRONMENTS

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OBJECTIVES

In this article, we deal with a specific aspect of the representation of particles by means of computing applications and how this relatively new way of representation is inserted into the scientific education of secondary school students. Firstly, we consider some general aspects of the representation in chemistry basing ourselves on the contributions of the teaching chemistry research community. Then, we discuss the representation of particles also getting support from some studies in the area of Science Education so that we can show the contributions of the studies about the use of the applications of visualization, with emphasis on the distinction between animations and simulations. In the second part, we describe the functionalities of the application in the construction of molecular objects that has been developed in our laboratory and their first use in secondary school classrooms.

THEORETICAL APPROACH

There is a certain consensus around the idea that the chemical knowledge is constructed by the combination of three dimensions of reality: macroscopic, microscopic and symbolic. Part of the phenomena and the chemical processes are perceptible and observable through sensorial information and measurements that are materialized in a macroscopic dimension. Within the atomic-molecular paradigm in force, in which the particle nature of the matter is the theoretical basis for the interpretation of these phenomena and processes, it is admitted another dimension of the reality in which the phenomena involving movement and interaction of particles occur. In a symbolic dimension, substances, particles and transformations are represented by means of symbols, formulas and chemical equations, as well as by algebraic expressions, being, therefore, a semiotic materialization of the reality.

The representation of levels of knowledge through multiple means has been efficient in chemistry teaching through the use of different systems of symbols to represent information in different ways. The superficial characteristics of each system of symbols can better represent certain characteristics of the information (Kozma and Russel, 1997).

Studies have shown good learning results when using concrete molecular objects as a way of visualizing the model of particles and the associated chemical transformations. Some authors have observed a cumulative effect of long term in the students´ understanding of the phenomena when submitted to the manipulation of these concrete molecular objects (Gabel and Sherwood, 1980). This type of visualization is pointed as one of the most used nowadays once it simplifies, illustrates and allows the exploration of the structure and of the associated chemical process. However, these objects are rigid and generally in limited quantity, which restricts its use to the representation of small molecules.

One of the functionalities of the computing applications is to show animations in the molecular level of the chemical phenomenon, which is not possible through other means of representation. The use of this technology as a teaching tool allows the visualization of dynamic animations projected three-dimensionally, which has helped students to represent symbolically the chemical processes and, therefore, to interpret the phenomenology in macroscopic and microscopic dimensions. This support to learning provided by computing technologies has been considered as a specific and especially useful characteristic of these means to represent the three dimensions of the chemical thought, as they have the quality of disposing the information in different symbolic systems, though coordinated. Multiple representations interconnected allow the student to visualize interactions between molecules and to understand the related chemical concepts.

A problem that students frequently face is the performance of tasks that require abilities of three-dimensional visualization, as well as three-dimensional visualization of molecules that are represented bi-dimensionally in books. There are evidences that this type of representation, especially when animated and dynamic, might refine students´ three-dimensional visualization. It is in this way that some authors have defended the integration between computing graphics and three-dimensional representation as an effective way of refining the ability of visualization in the teaching of sciences (Barnea and Dori, 1999).

The use of virtual molecular objects generated by computers, besides permitting the arrangement of multiple representations which are coordinated and three-dimensionally projected, also favours varied types of manipulation of these objects, such as translation, rotation, size augment or reduction. Another advantage of computing visualization is the possibility of representing molecules of, virtually, any size, depending only on the capacity of the computer processing. In this sense, the development of computing applications for teaching activities appears as a potentially transforming alternative of school practices and of knowledge construction between students, once one considers the correlation of the three dimensions of chemical knowledge in the organization of activities and one investigates the rules of the actions mediated by the applications that are fundamentally different from those performed in teaching situations anchored in the experimentation or any other way of access to the phenomenology; this is so because the statute of the phenomenon alters radically when it is shifted from the bench to the computer screen (Giordan, 1999).

Let us consider some specificities of the representation of molecular objects in the computer taking into consideration two distinct ways of visualizing them: the animation and the simulation.

Computing animations are generated from general graphic edition applications, without necessarily including empirical values of properties of the substances or of the transformations obtained in scientific research, and they intend to emphasize certain superficial macroscopic or microscopic characteristics without obeying time or size scales. On the other hand, the computing simulations are generated from specific applications for the study of properties of the substances and chemical transformations, and are closely related to the environment of scientific research. To perform these simulations, theoretical or empirical values of chemical properties, such as angles and bond distances, are used, and time and size scales are parameterized in mathematical equations, which satisfy the physical laws that describe the phenomena.

An important outcome of the manipulation of several ways of representation is the possibility of creating a linking effect between the variable -theoretical nature - and the way of representing the property - imagetic nature. The visualization of molecular objects mediated by computer seems, therefore, to promote the linking between the simulation of a property of the molecule and its representation in the same envi-

ronment. This is a situation of high didactic value capable of mobilizing the students´ actions in the manipulation of objects, in the discursive elaboration and also in the meaning construction, as we have discussed somewhere (Giordan, 2004).

In spite of the fact that there are several tools for the visualization and construction of virtual molecular objects aimed at researchers, the use of these tools by secondary school students and even by university freshmen in chemistry is hindered due to the depth of knowledge involved in the calculus and in the control of variables. In some cases, the students have to supply values to variables such as force constants of chemical bonds, to know details about the process of minimizing the energy or else details about the organization of output information produced by the applications. Thus, having access to the applications of molecular visualization based on simulations, it is necessary to develop tools that simplify data transfer between input and output interfaces, and simultaneously make it possible to students to take control over variables that affect visualization.

THEMATIC DEVELOPMENT

Construtor is a tool for the creation of virtual molecular objects that use the hypertext transfer protocol (http) to perform the communication of the Client with the Server. Through this interface the student can build animations of bi-dimensional molecular models, and also build and visualize simulations of these models three-dimensionally projected from the condensed structural formula by means of a plug-in. The animations and the simulations are disposed on the same screen so that the student has the opportunity to compare his own representations with the representations associated with the model scientifically accepted. The simulations are done using a molecular modelling package, and visualized with a *plug-in* Chime®, both applications of public domain and highly used in the scientific field.

The environment of graphic animation was written with the help of the application Flash®, from Macromedia, which is an application of general use in the construction of graphic animations. In this application, bi-dimensional designs can be created from simple geometric figures. The tools provide options in which the draws can simulate the visual sensation of three-dimensionality. The draws are created in a varied quantity of pictures with different dispositions, so that the overlap of pictures creates a visual sensation of movement. The possibility of creating different draws in separated layers as part of the same animation, favours an environment of organized and planned edition.

The program running in the Server, which interacts with the user environment of three-dimensional simulation and provides appropriate files for visualization was written in C language ANSI pattern to be run in the Server with the environment GNU/Linux, from RedHat/Fedora distribution. This part of the environment provides an input box for the user to send to the Server, through the communication protocol via the Internet hypertext, a sequence of letters and numbers correspondent to a condensed structural formula of an organic molecule, such as $CH_3CH_2CH_3$, CH_3CH_2CHO, $CH_3CH_2COCH_3$ or $CH_3OCH_2CH_3$, inclusively with branched, unsaturated and cyclic chain.

A simple test of usability of the Construtor program was done in a public school with 32 students of year eleven class in the State of São Paulo, Brasil, aiming at collecting information to improve the present version. The students had access to the Construtor program using an Organic Chemistry Tutorial (OCT) as instructional supporting material, which was used as class guidance activity.

A usability test has been carried out using a methodology developed in our laboratory. We have recorded the students with a webcam and the computer screen has been captured with a software when they were working around the computer. The webcam was placed in a position to record the reactions of the students before what was proposed and presented. Both images of the students and the screen have been acquired in synchronized mode. A second webcam might be added to record the interaction of the students with the computer screen. Each one of the recorded images were stored in different computer files, which were used

to analyse the actions of the students. In this methodology, the synchronized images are displayed in just one computer window what permits the researcher to visualize the whole interaction. Another field might be added in the bottom of the computer window presenting the transcriptions of the speech.

In these classes, the students had positive attitudes both towards the material and the activities, even those who did not actively participate in similar activities without the use of computers. A illustrative speech of a female student reveals some aspects to be further analysed:

> "Before that I saw something ... molecules, something unseen with the eyes and then it was somehow … a daydream, guys don't know what it really is. Now guys work in solid basis, visually, turning molecules, this becomes a concret stuff. Guys image, guys seen an object and tell: Jesus! It is set like this, that way, that bond. That's new stuff. From that moment guys see chemistry with new eyes, a concret stuff, in place of image stuff. And this gona be very useful in our school life."

The students´ answers to the activities and to the proposed questions brought forth evidences of mastering the symbolical systems for the model of particles when interpreting the macroscopic phenomena and properties. In general, the students showed good performance when using the interfaces and no operational difficulty with the animation and simulation interfaces was observed. More refined usability tests are been planned from the data of screen register, simultaneously with their audiovisual register of the students, before we start studying aspects of the action performed and of the meaning construction.

CONCLUSIONS

In general, the students showed good performance when using the interfaces and no operational difficulty with the animation and simulation interfaces was observed. More refined usability tests have been planned to improve the methodology of synchronic recording of both computer screen and students. After that, we will be ready for investigating meaning construction and interaction around the computer.

Another phase of the project centres in the development of an interface for visualization based on the Java 2 platform and using a API JOGL (*Java bindings for OpenGL*), in order to incorporate movements that mimetize the movement of atomic vibration besides the functionalities already available in *Chimie*®. We now study the possibility of converting the bidimensional data from representations of molecular objects, drawn in the animation interface, into input data to the simulation interface. This will offer an option for the creation of objects to manage the input data without information on the condensed structural formula. This interface of direct conversion might be used by university students who have already mastered chemical symbolical systems in high degree.

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